A least squares method for Laplace's equation with Dirichlet boundary conditions

By P. Jarratt and C. Mack*

A technique is given for solving certain partial differential equations in regions whose boundaries are formed from polygonal lines or arcs of some simple curves. The method is simple to apply and is attractive when solutions are required for a variety of related boundary configurations.

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1. Introduction

In this paper a method for solving Laplace's or Poisson's equation is described for cases where the function is specified on the boundary. The method depends on fitting a linear combination of known solutions by least squares to the boundary conditions, and in cases where the boundaries are composed of straight lines, or arcs of circles and ellipses, it is shown that the normal equations can be rapidly set up by means of recurrence relations. For problems of this kind, which arise frequently in practice, the approach we have used appears to possess a number of significant advantages over the more usual finite difference techniques.

2. Illustrative problem and basic method

We consider the problem of determining ψ satisfying the Poissonian Equation

$$\frac{\partial^2\psi}{\partial r^2}+\frac{1}{r}\frac{\partial\psi}{\partial r}+\frac{1}{r^2}\frac{\partial^2\psi}{\partial\theta^2}=-2, \qquad (2.1)$$

in a region R and subject to the condition $\psi = 0$ on the boundary S. The solution of (2.1) is of the form

$$\psi = -\frac{r^2}{2}+\phi, \qquad (2.2)$$

where the first term on the right of (2.2) is a particular integral for (2.1) and ϕ, the solution of Laplace's equation, can be written

$$\phi = A_0 + \sum_{n=1}^{\infty} r^n(A_n \cos n\theta + B_n \sin n\theta), \qquad (2.3)$$

for some circle of convergence and origin inside the boundary.

We now obtain an approximate solution of (2.1) by truncating the series (2.3) for ϕ at the mth terms and minimising $\int_s \psi^2 ds$, the resulting normal equations having the form

$$\sum_{k=0}^{m}\alpha_{j,k}A_k + \sum_{k=1}^{m}\beta_{j,k}B_k = C_j, \quad j = 0, 1, \ldots, m$$

$$\sum_{k=0}^{m}\beta_{k,j}A_k + \sum_{k=1}^{m}\gamma_{j,k}B_k = S_j, \quad j = 1, 2, \ldots, m$$

where

$$\alpha_{j,k} = \int_s r^{j+k}\cos j\theta \cos k\theta ds,$$

$$\beta_{j,k} = \int_s r^{j+k}\cos j\theta \sin k\theta ds,$$

$$\gamma_{j,k} = \int_s r^{j+k}\sin j\theta \sin k\theta ds,$$

$$C_j = \tfrac{1}{2}\int_s r^{j+2}\cos j\theta ds,$$

$$S_j = \tfrac{1}{2}\int_s r^{j+2}\sin j\theta ds. \qquad (2.4)$$

Now in many practical problems, the boundary s is formed from a small number of simple curves, and we shall show that in certain cases it is possible to evaluate the integrals (2.4) rapidly from recurrence relations.

3. Straight line boundaries

In **Fig. 1**, 0 is the origin and P the point (r, θ) on the straight line AB. From the figure we obtain immediately

$$r = a \sec(\theta - \alpha),\ ds = a \sec^2(\theta - \alpha)d\theta. \qquad (3.1)$$

If now we define

$$I_{M,N} = C_{M,N} + iS_{M,N} = \int_{AB}\sec^M(\theta - \alpha)e^{iN\theta}d\theta, \qquad (3.2)$$

we find, by substituting the relations (3.1) in the expression for $\alpha_{j,k}$ and using the sine and cosine addition

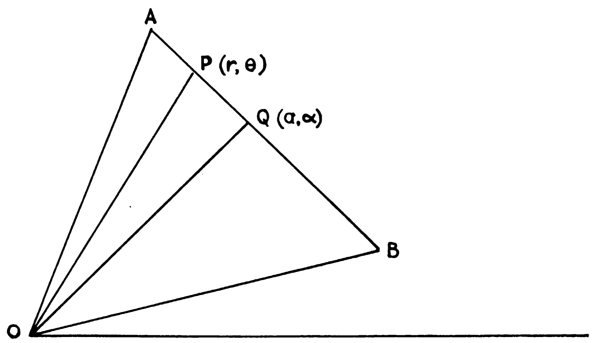

Fig. 1

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formulae, the result

$$\alpha_{j,k} = \tfrac{1}{2}a^{j+k+1}[C_{j+k+2,\,j+k} + C_{j+k+2,\,j-k}].$$

Also by integrating (3.2) twice by parts we obtain the recurrence

$$(N^2 - M^2)I_{M,N} = e^{iN\theta}\sec^{M+1}(\theta - \alpha)[M\sin(\theta - \alpha) - iN\cos(\theta - \alpha)] - M(M+1)I_{M+2,N}. \quad (3.3)$$

Hence

$$(N^2 - M^2)C_{M,N} = \sec^{M+1}(\theta - \alpha)[M\sin(\theta - \alpha)\cos N\theta + N\cos(\theta - \alpha)\sin N\theta] - M(M+1)\,C_{M+2,N}, \quad (3.4)$$

and by setting $M = N$ we also have

$$C_{M+2,\,M} = \sec^{M+1}(\theta - \alpha)\sin[(M+1)\theta - \alpha]/(M+1). \quad (3.5)$$

We now show how these results may be used to generate the various contributions to the least squares matrix. The values of $\alpha_{j,\,k}$ required are those occurring in the symmetric array

be obtained by computing the quantity $E_m = \int_s \psi^2 ds$, and using (3.1) and the minimum conditions, this can be written for the segment AB as

$$E_m = \frac{a^3}{2}\left\{\frac{a^2}{2}C_{6,\,0} - \left[A_0C_{4,\,0} + \sum_{j=1}^{m} a^j(A_jC_{j+4,\,j} + B_jS_{j+4,\,j})\right]\right\}.$$

Since the terms in this expression must all be found in constructing the least squares matrix, E_m can be computed as soon as the set of A_j, B_j has been obtained.

It is also possible to assign an upper limit to the error in ψ, for suppose ϕ_m is an approximation to the true value of ϕ given by (2.3), then $\phi_m - \phi$ is also a solution of Laplace's equation. Furthermore, since the maximum value of a solution always occurs on a boundary, the maximum departure of the finite approximation to ψ from zero on the boundary will give the maximum error anywhere.

$$\alpha = \begin{bmatrix} C_{2,\,0} & C_{3,\,1} & C_{4,\,2} & & C_{m+2,\,m} \\ & (C_{4,\,2} + C_{4,\,0}) & (C_{5,\,3} + C_{5,\,1}) & \cdots & (C_{m+3,\,m+1} + C_{m+3,\,m-1}) \\ & & (C_{6,\,4} + C_{6,\,0}) & \cdots & (C_{m+4,\,m+2} + C_{m+4,\,m-2}) \\ & & & \ddots & \vdots \\ & & & & (C_{2m+2,\,2m} + C_{2m+2,\,0}) \end{bmatrix}$$

where for convenience the factors $\frac{1}{2}a^{j+k+1}$ have been omitted.

First, $C_{2,\,0}$ is easily found by setting $M = 0$ in (3.5), and the sequence $C_{4,\,0}$, $C_{6,\,0}, \ldots, C_{2m+2,\,0}$ can then be generated using (3.4). Similarly $C_{3,\,1}$ is computed from (3.5), enabling us to obtain the elements $C_{5,\,1}$, $C_{7,\,1}, \ldots, C_{2m+1,\,1}$, and in a like fashion we find all the terms in the array except for the sequence $C_{m+2,\,m}$, $C_{m+3,\,m+1}, \ldots, C_{2m+2,\,2m}$ in the last column. However, these are immediately available by repeated use of (3.5). A precisely similar treatment enables us to obtain the values of $\beta_{j,\,k}$, while an examination of $\gamma_{j,\,k}$ shows that these elements consist of values which have already been computed in finding the $\alpha_{j,\,k}$. Again, $C_j = \frac{1}{2}a^{j+3}C_{j+4,\,j}$, $S_j = \frac{1}{2}^{j+3}S_{j+4,\,j}$ and these also will have been found in the computation of the $\alpha_{j,\,k}$ and $\beta_{j,\,k}$, apart from C_m and S_m. However, since $C_{m+2,\,m}$ and $S_{m+2,\,m}$ are already available, this causes no difficulties.

If, as is often the case, the boundary S is composed entirely of straight lines, then by integrating over each segment and accumulating the results, the coefficients for the set of A_j and B_j can be simply found. In a computer program the same logic will suffice to obtain the contribution from each segment and results for various boundary configurations can be obtained by altering the parameters a and α appropriately.

A measure of the accuracy of the approximation can

In the case where a particular choice of m yields insufficient accuracy, the next higher order approximation can make use of much of the previous calculation and the new solution found with relative economy.

It is also worth noting that in problems where the variation of ψ on the boundary is of the form $h(r\cos\theta, r\sin\theta)$, the approach we have used can again be applied. The extension to the case where h is a constant is particularly simple.

4. Circular arcs

We now consider the situation where a segment of the boundary is formed from an arc of a circle.

In **Fig. 2**, 0 is the origin, C the centre of the circular

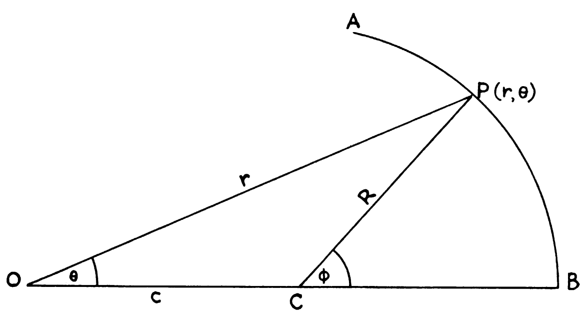

Fig. 2

arc and R its constant radius. Considering again the basic integrals (2.4), it is easy to see that these can all be found provided we can evaluate integrals of the type

$$E_{M,N} = C_{M,N} + iS_{M,N} = \int_s r^M r^{2N} \exp(Mi\theta) ds. \quad (4.1)$$

From Fig. 2 we have $ds = Rd\phi$, and defining $a = R\exp(i\phi) + c = r\exp(i\theta)$, $b = R\exp(-i\phi) + c = r\exp(-i\theta)$, we find we can write (4.1) as

$$E_{M,N} = R\int_s a^{M+N} b^N d\phi. \quad (4.2)$$

Using $ad\phi = -ida + cd\phi$ and integrating (4.2) by parts we have

$$ME_{M,N} = -iRa^{M+N}b^N - NcE_{M+1,\,N-1} + c(M+N)E_{M-1,\,N}, \quad (4.3)$$

and for $N = 0$ this reduces to

$$ME_{M,\,0} = -iRa^M + McE_{M-1,\,0} \quad (4.4)$$

Fig. 2 also gives us the relation

$$r^2 = R^2 - c^2 + rc\,[\exp(i\theta) + \exp(-i\theta)]$$

and using this in (4.1) yields the recurrence

$$E_{M,N} = (R^2 - c^2)E_{M,\,N-1} + cE_{M+1,\,N-1} + cE_{M-1,\,N}. \quad (4.5)$$

(4.3) and (4.5) may now be combined to give

$$NcE_{M-1,\,N} = iRa^{M+N}b^N + c(M+N)E_{M+1,\,N-1} + M(R^2 - c^2)E_{M,\,N-1} \quad (4.6)$$

In each case the appropriate recurrences for $C_{M,\,N}$ and $S_{M,\,N}$ are readily obtained. It is again interesting to see how the elements of the least squares matrix can be generated. In this case the values of $\alpha_{j,k}$ necessary are those which occur in the array

$$\alpha = \begin{bmatrix} c_{0,\,0} & c_{1,\,0} & c_{2,\,0} & & c_{m,\,0} \\ & \tfrac{1}{2}(c_{2,\,0} + c_{0,\,1}) & \tfrac{1}{2}(c_{3,\,0} + c_{1,\,1}) & \cdots & \tfrac{1}{2}(c_{m+1,\,0} + c_{m-1,\,1}) \\ & & \tfrac{1}{2}(c_{4,\,0} + c_{0,\,2}) & \cdots & \tfrac{1}{2}(c_{m+2,\,0} + c_{m-2,\,2}) \\ & & & \ddots & \vdots \\ & & & & \tfrac{1}{2}(c_{2m,\,0} + c_{0,\,m}) \end{bmatrix}$$

Now with the starting value $c_{0,\,0} = [R\phi]_s$, we can use (4.4) to generate successively

$$c_{1,\,0}, c_{2,\,0}, \ldots, c_{2m,\,0}. \quad (4.7)$$

Next by using $c_{1,\,0}$ and $c_{2,\,0}$ in (4.6) we can find $c_{0,\,1}$, and similarly by selecting successive pairs of values from the sequence (4.7) we obtain

$$c_{1,\,1}, c_{2,\,1}, \ldots, c_{m-1,\,1}. \quad (4.8)$$

The next row of α is generated using (4.6) and successive pairs of values from the sequence (4.8), and the process continues until all the elements of α have been found. As in the case of straight line boundaries, the same technique also applies to find the $\beta_{j,\,k}$ and the $\gamma_{j,\,k}$, C_j and S_j are again composed of terms already computed for α and β.

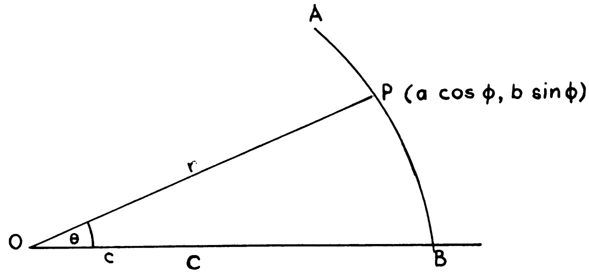

Fig. 3

5. Elliptic arcs

In **Fig. 3**, P is a point with parametric coordinates $(a\cos\phi, b\sin\phi)$ on an ellipse centre C.

In the case of elliptic boundaries it is convenient to minimise not $\int_s \psi^2 ds$ but $\int_s w\psi^2 ds$ where w, a weighting factor, is chosen to simplify the evaluation of integrals of the types (2.4). If now we write $A = r\exp(i\theta)$, $b = r\exp(-i\theta)$ and set $w = d\phi/ds$, we find these integrals can be computed provided we can evaluate

$$E_{M,N} = C_{M,\,N} + iS_{M,\,N} = \int_s A^M B^N d\phi. \quad (5.1)$$

Using the relations $r\cos\theta = a\cos\phi + c$, $r\sin\theta = b\sin\phi$, we have $A = d/d\phi(a\sin\phi - ib\cos\phi) + c$, and hence (5.1) can be written

$$E_{M,\,N} = \int_s A^{M-1}B^N d(a\sin\phi - ib\cos\phi)d\phi + cE_{M-1,\,N}. \quad (5.2)$$

By integrating (5.2) by parts we obtain after some manipulation the recurrence

$$\begin{aligned}(M+N)E_{M,\,N} = {} & A^{M-1}B^N(a\sin\phi - ib\cos\phi) \\ & + (M-1)(a^2 - b^2 - c^2)E_{M-2,\,N} \\ & + c(2M+N-1)E_{M-1,\,N} \\ & + N(a^2 + b^2 - c^2)E_{M-1,\,N-1} + NcE_{M,\,N-1}\end{aligned} \quad (5.3)$$

and setting $N = 0$ gives

$$ME_{M,\,0} = A^{M-1}(a\sin\phi - ib\cos\phi) + (M-1)(a^2 + b^2 - c^2)E_{M-2,0} + c(2M-1)E_{M-1,0} \quad (5.4)$$

Now in this case the array α is given by

$$\alpha = \begin{bmatrix} c_{0,0} & c_{1,0} & c_{2,0} & \cdots & c_{m,0} \\ & \tfrac{1}{2}(c_{2,0}+c_{1,1}) & \tfrac{1}{2}(c_{3,0}+c_{2,1}) & \cdots & \tfrac{1}{2}(c_{m+1,0}+c_{m,1}) \\ & & \tfrac{1}{2}(c_{4,0}+c_{2,2}) & \cdots & \tfrac{1}{2}(c_{m+2,0}+c_{m,2}) \\ & & & & \vdots \\ & & & & \tfrac{1}{2}(c_{2m,0}+c_{m,m}) \end{bmatrix}$$

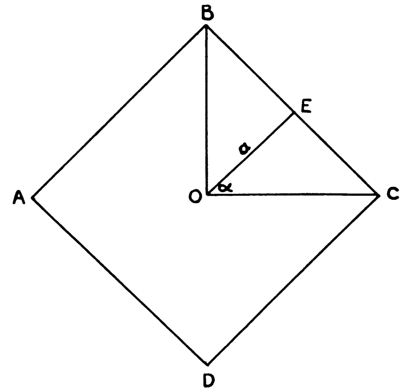

Fig.4.

We easily find $c_{0,0} = [\phi]_s$, $c_{1,0} = [a \sin \phi + c\phi]_s$, and hence using (5.4) we can generate $c_{2,0}, c_{3,0}, \ldots c_{2m,0}$. We also note from (5.1) and the definitions of A and B that $E_{M,N} = \bar{E}_{N,M}$ where $\bar{E}_{M,N}$ is the complex conjugate of $E_{M,N}$. Thus integrals of the form $c_{0,1}, c_{0,2}, \ldots$, can be simply evaluated once the corresponding $c_{1,0}, c_{2,0}, \ldots$, have been found. For example, using the real part of (5.3) with $M = N = 1$ to find $c_{1,1}$, we see we require $c_{0,1}$, $c_{0,0}$ and $c_{1,0}$, which are all available. Similarly for $c_{2,1}$ we find we need $c_{0,1}$, $c_{1,1}$, $c_{1,0}$ and $c_{2,0}$ and again these have all been computed. In this way we may build up all the elements of the array α and $\beta_{j,k}$, $\gamma_{j,k}$, C_j and S_j are again found as in the cases of straight line and circular boundaries.

6. A numerical illustration

For the purpose of a numerical example we consider the problem of solving (2.1) in the square $ABCD$ shown in **Fig. 4** in which $\alpha = 45°$ and $a = 1$. We make use of the symmetry of the problem to set $\psi = -r^2/2 + \phi$ where

$$\phi = a^2 \sum_{n=0}^{m} (r/a)^{4n} A_n \cos 4n\theta, \tag{6.1}$$

and where the form of ϕ has been altered slightly to control the growth of numbers in the solution, and we investigate the solution of (2.1) in the triangle OCE for which θ varies from 0 to $\pi/4$.

The problem was solved for $m = 0, 1, 2$ and 3 and in each case the quantity E_m and the values of ψ on the boundary, representing the errors, were calculated. In **Table 1** we show the solution vectors $[Ai]$, $i = 0, 1, 2, 3$. The calculation of ψ along the boundary CE showed that the errors e_m are well approximated by the first neglected term of (6.1), the maximum value Max e_m occurring, as expected, at the node C. In **Table 2** we give the values of $E_m = \int_0^{\pi/4} \psi^2 ds$, together with those of Max e_m for $m = 0, 1, 2, 3$.

7. Discussion

The method developed in this paper belongs to a class of techniques known as analytic methods as opposed to finite difference approximations. In common with most other methods of its type, the least squares approach we have discussed is limited to a special class of problems, but where it is applicable it may enjoy a number of advantages over the more general finite difference methods. For example, in the problem treated here an

Table 1

A \ m	0	1	2	3
A_0	$6\cdot667 \times 10^{-1}$	$5\cdot891 \times 10^{-1}$	$5\cdot894 \times 10^{-1}$	$5\cdot894 \times 10^{-1}$
A_1		$9\cdot698 \times 10^{-2}$	$9\cdot077 \times 10^{-2}$	$9\cdot122 \times 10^{-2}$
A_2			$2\cdot631 \times 10^{-3}$	$1\cdot754 \times 10^{-3}$
A_3				$2\cdot436 \times 10^{-4}$

Table 2

m	0	1	2	3
E_m	$2\cdot222 \times 10^{-2}$	$5\cdot748 \times 10^{-5}$	$1\cdot830 \times 10^{-6}$	$1\cdot981 \times 10^{-7}$
Max e_m	$-3\cdot333 \times 10^{-1}$	$-2\cdot299 \times 10^{-2}$	$-5\cdot467 \times 10^{-3}$	$-2\cdot083 \times 10^{-3}$

error estimate for the solution was readily obtained and the solution of the same problem for a variety of related boundary configurations would have presented few difficulties. From the standpoint of computing effort, a choice between the two classes of method is not obvious and will not always be made in the same direction.

In applying the method we have not so far experienced the traditional difficulties associated with least squares. However, the problems we have solved have been simple and difficulties may well arise for larger values of m. These would be needed when the solution exhibits poor behaviour near some points, for example in the neighbourhood of re-entrant corners or discontinuous boundary conditions. The recurrence relations themselves which are used to generate the least squares matrix have proved numerically stable in the cases we have examined.

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A new method for solving polynomial equations

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An iterative method for finding the zeros of a polynomial $f(z)$ is given, based on approximating $f(z)/f'(z)$ by a bilinear form. The method has high order convergence for both simple *and* repeated zeros (whatever the multiplicity) and takes very few iterations (average < 15) per zero however 'difficult' the polynomial.

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1. Introduction

The problem of determining numerically all the zeros of a polynomial equation is of great practical importance in science and engineering. However, it has proved difficult to devise a method which works equally well for all polynomials (whether coefficients are real or complex, whether zeros are distributed, clustered or repeated etc.). Wilkinson's (1959) paper discusses the difficulties and gives an assessment of a number of established methods (general accounts have also been given by Hochstrasser (1962) and Bareiss (1959)).

In this paper a new iterative method is presented which has proved extremely successful in solving polynomials whether difficult or not. It is *not affected* by the multiplicity of the zero unlike Bairstow's method (1914), which is impractically slow in finding a double zero (or two 'clustered' zeros), as is Muller's method (1956) when the order of multiplicity is three (or there are three 'clustered' zeros). A further advantage of our method is that at each stage of the iteration the best of three alternatives is chosen and this reduces the incidence of 'cycling' (a possibility with all iterative methods), and no case of cycling has yet been observed. A novel technique for starting the iteration has led to rapid solution with the zero found at each iteration often the smallest and, practically always, of lower than average modulus. The iteration is 'signed off' in a novel manner, yielding high accuracy. The theory of the method is now described (together with a generalisation); operational details follow, and actual examples conclude the paper.

2. Theory of the unmodified method

We use the same idea as Jarratt and Nudds (1965) but we apply it not to $f(z)$ but to $f(z)/f'(z)$. Thus near a zero α of an nth degree polynomial $f(z)$, we can write

$$1/F(z) \equiv f(z)/f'(z) \doteqdot (z-a)/(b+cz), \qquad (2.1)$$

where $f'(z)$ is the derivative of $f(z)$. This is true even if α is a repeated zero when $f'(z)$ will also have a zero at α. Thus, if $f(z) = A(z-\alpha)^r(z-\beta)(z-\gamma)\ldots$, then $F(z) = r/(z-\alpha) + 1/(z-\beta) + 1/(z-\gamma) + \ldots$, so that if z is close to α, we have

$$1/F(z) = (z-\alpha)/[r + (z-\alpha)\{1/(\alpha-\beta) + 1/(\alpha-\gamma) + \ldots\} + O(z-\alpha)^2].$$

If now we write $f'(z_i)/f(z_i) \equiv F_i$ (2.2)

and we have three values of z_i, namely z_1, z_2, z_3 then (2.1) and (2.2) combined give the simultaneous equations

$$b + cz_i + aF_i = z_iF_i,\ i = 1, 2, 3. \qquad (2.3)$$

Hence by solving the set (2.3) for a we obtain an estimate of α. We can now put $z_4 = a$ and solve (2.3) with $i = 2, 3, 4$, thereby finding a new value of a, and so on. If the process converges, then a converges to α.

From (2.3) we easily find the symmetric formula

$$a = \frac{z_1F_1(z_2-z_3) + z_2F_2(z_3-z_1) + z_3F_3(z_1-z_2)}{F_1(z_2-z_3) + F_2(z_3-z_1) + F_3(z_1-z_2)}, \qquad (2.4)$$

which shows that the value of a is independent of the order of z_1, z_2 and z_3. However, in numerical work, the use of (2.4) leads to a serious loss of significant figures

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