

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 n th degree polynomial $f(z)$, we can write

$$1/F(z) \equiv f(z)/f'(z) \div (z - \alpha)/(b + cz), \quad (2.1)$$

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 $f(z) = A(z - \alpha)^r(z - \beta)(z - \gamma) \dots$, then $F(z) = r/(z - \alpha) + 1/(z - \beta) + 1/(z - \gamma) + \dots$, so that if z is close to α , we have

$$1/F(z) = (z - \alpha)/[r + (z - \alpha)\{1/(\alpha - \beta) + 1/(\alpha - \gamma) + \dots\} + O(z - \alpha)^2]. \quad (2.2)$$

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

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

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

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

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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and we do better to compute a as a correction to z_3 from the formula

$$a = z_3 + (z_2 - z_3)(z_3 - z_1)(F_2 - F_1)/\{(z_3 - z_2)(F_2 - F_1) + (z_1 - z_2)(F_3 - F_2)\}. \quad (2.5)$$

If now $\alpha, \beta, \gamma, \dots$, are the zeros of $f(z)$, then algebraic manipulation shows that

$$a = \frac{\alpha/\{(z_1 - \alpha)(z_2 - \alpha)(z_3 - \alpha)\} + \beta/\{(z_1 - \beta)(z_2 - \beta)(z_3 - \beta)\} + \dots}{1/\{(z_1 - \alpha)(z_2 - \alpha)(z_3 - \alpha)\} + 1/\{(z_1 - \beta)(z_2 - \beta)(z_3 - \beta)\} + \dots} \quad (2.6)$$

The corresponding result when some of the zeros are repeated is obvious. Hence if we define $z_i - \alpha = \epsilon_i$, $i = 1, 2, 3, 4$, and all the ϵ_i are small compared with $\alpha - \beta$, $\alpha - \gamma, \dots$, then we see from (2.6) that

$$\epsilon_4 = H\epsilon_1\epsilon_2\epsilon_3 \quad (2.7)$$

where H is approximately a constant. Difference equations of the type (2.7) are well known and it is readily shown from (2.7) that the order of the method is the real root of the equation $t^3 = t^2 + t + 1$, namely 1.839. Moreover this is true irrespective of whether the root is simple or repeated.

Again, if z_1, z_2, z_3 are all large compared with $\alpha, \beta, \gamma, \dots$, then

$$a \doteq (\alpha + \beta + \gamma + \dots)/(1 + 1 + 1 + \dots) = (\alpha + \beta + \gamma + \dots)/n. \quad (2.8)$$

Thus if three estimates remote from the zeros are taken, the next approximation is located at the centroid of the zeros. This would seem to be a very valuable property of the method.

Although the formula (2.5) works very well, we did in practice introduce two modifications. The first of these was aimed at eliminating the occasional unfortunate situation in which the denominator of (2.5) is fortuitously zero, or very nearly so, and the second improved the accuracy of the final estimate of α . These modifications are described in the following section.

3. Theory of the modified method

If we apply the method of (2.1) to finding a zero, not of $f(z)$, but of $\psi(z) = f(z)/z^n$, we arrive at the iterative formula

$$a' = z_3 + \frac{(z_1 - z_3)(z_2 - z_3)\{n(z_2 - z_1) + z_1^2F_1 - z_2^2F_2\}}{(z_2 - z_3)\{z_1^2F_1 - z_2^2F_2\} + (z_1 - z_2)\{z_3^2F_3 - z_2^2F_2\}}. \quad (3.1)$$

Thus a' can be computed at the same time as a and involves no extra evaluations of the polynomial. Furthermore we may now choose for z_4 whichever of a or a' is nearer z_3 .

We can show by algebraic manipulation that

$$a' = \frac{\alpha^3/(z_1 - \alpha)(z_2 - \alpha)(z_3 - \alpha) + \beta^3/(z_1 - \beta)(z_2 - \beta)(z_3 - \beta) + \dots}{\alpha^2/(z_1 - \alpha)(z_2 - \alpha)(z_3 - \alpha) + \beta^2/(z_1 - \beta)(z_2 - \beta)(z_3 - \beta) + \dots} \quad (3.2)$$

It is extremely unlikely that the denominators of both (2.5) and (3.1) will be simultaneously zero. Hence the chance of this affecting the iterative process is virtually eliminated.

We also note that since we have to compute $1/F_i = f(z_i)/f'(z_i)$, $i = 1, 2, 3$, for formulae (2.5) and (3.1), we can use, at no extra cost, the Newton–Raphson formula in the form

$$a'' = z_3 - 1/F_3, \quad (3.3)$$

and take whichever of a, a', a'' is the nearest to z_3 as our value of z_4 . Now when the estimates are very close to the true value α , the computation of both a and a' may involve much cancellation and rounding off errors may be appreciable. These errors will be least in computing a'' and, if the zero α is isolated, a'' will give us the greatest final accuracy.

Another important advantage of alternative choices concerns the fact that some iterative methods occasionally fail in the sense of ‘cycling’ round a series of values of z_i without $f(z_i)$ converging to zero. We have observed this phenomenon with both Muller’s (1956) and Bairstow’s (1914) methods and also in one instance with our unmodified method (Section 2). The modified version (Section 3), however, has not cycled in any of the cases tried and this is probably due to the fact that, at each iteration, one of three alternatives is chosen.

4. Generalisation of the method

It is possible to consider a more general form than (2.1), namely

$$1/F(z) \equiv f(z)/f'(z) \doteq (z - a)/\{c_0 + c_1z + c_2z^2 + \dots + c_{k-2}z^{k-2}\}. \quad (4.1)$$

Here, given the k points (z_i, F_i) , $i = 1, 2, \dots, k$, we solve the simultaneous equations

$$aF_i + c_0 + c_1z_i + c_2z_i^2 + \dots + c_{k-2}z_i^{k-2} = z_iF_i, \quad (4.2)$$

$i = 1, 2, \dots, k$. The value of a gives us z_{k+1} , and we then solve (4.2) for $i = 2, 3, \dots, k + 1$, and so on.

It can be shown that

$$a = \frac{\alpha/\{z_1 - \alpha)(z_2 - \alpha) \dots (z_k - \alpha)\} + \beta/\{z_1 - \beta)(z_2 - \beta) \dots (z_k - \beta)\} + \dots}{1/\{z_1 - \alpha)(z_2 - \alpha) \dots (z_k - \alpha)\} + 1/\{z_1 - \beta)(z_2 - \beta) \dots (z_k - \beta)\} + \dots} \quad (4.3)$$

where $\alpha, \beta, \gamma, \dots$, are the zeros of $f(z)$.

The iteration rule is

$$z_{m+1} = z_m + (z_{m-k+1} - z_m)(z_{m-k+2} - z_m) \dots (z_{m-1} - z_m)A_{m, k-1}/A_{m, k} \quad (4.4)$$

where

$$A_{m, 1} = F(z_{m-1}), A_{m, 2} = A_{m, 1} - A_{m+1, 1},$$

$$A_{m, k+2} = (z_{m-k} - z_m)(z_{m-k+1} - z_m) \dots$$

$$(z_{m-1} - z_m)A_{m-1, k+1}$$

$$-(z_{m-k-1} - z_{m-k})(z_{m-k-1} - z_{m-k+1}) \dots (z_{m-k-1} - z_{m-1})A_{m, k+1} \quad (4.5)$$

The case $k = 2$, gives the secant formula; $k = 3$ gives formula (2.5); $k = 4$ increases the order of convergence marginally to 1.928 but at the cost of some cancellation of significant figures, increase of rounding errors, a slightly slower operation, and increase in length of program.

We decided that, taking all considerations into account, $k = 3$ gave the best working form.

5. Operational details

We have to find a set of initial values for z_1, z_2, z_3 . Now, if

$$f(z) = a_0 z^n + a_1 z^{n-1} + \dots + a_{n-1} z + a_n \quad (5.1)$$

then one zero, at least, has a modulus less than or equal to

$$|a_n/a_0|^{1/n} = 5w, \text{ say.} \quad (5.2)$$

So we start with $+iw, -w + iw, +2iw$. If after 50 iterations we are not near a zero, we restart with $+2iw, -w + 2iw, -w + 3iw$; and if this fails we take 3 more points inside the circle $|z| = 5w$, etc. However, 3 real or 3 imaginary values are best avoided as then all subsequent z_i may be real or imaginary. In practice, we have *never* failed to find a zero within the prescribed number of iterations with the first set.

After a zero α has been found, we recalculate (5.2) for the reduced polynomial $f(z)/(z - \alpha)$ and start with

$$-w \pm iw, -w \pm 2iw, \bar{\alpha} \quad (5.3)$$

where $\bar{\alpha}$ is the conjugate of α and *all* the imaginary parts in (5.3) have the same sign. Where zeros are in conjugate pairs this speeds up the process and does so particularly where there are repeated or clustered zeros.

The initial values z_1, z_2, z_3 can be rearranged in descending order of $|f(z_i)|$. This ensures that the z_i with lowest $|f(z_i)|$ appears in the first three iterations.

We sign off thus: In single-length arithmetic we continue calculating $f(z_i)$ until $|f(z_i)| < 10^{-9}|a_n|$. (We work on an I.C.T. 1909 computer with a 36 bit mantissa equal to about 11 decimal places; any number between 0.1 and $1 \times 10^{-9}|a_n|$ will probably do. This stage is usually reached well before the 50th iteration with our

method.) We then continue recording the lowest $|f(z_i)|$ so far obtained until two successive $|f(z_i)|$ are greater than this value. The corresponding z_i is taken as the correct value of the zero. $f(z)$ is divided by $z - z_i$ and a zero of the quotient is then found.

6. Numerical results

In what follows, the zeros are all given in order of appearance using our method; the first wrong digit is underlined and the number of iterations is given in brackets after each zero.

6.1. Single-length arithmetic

Dimsdale (1948) gave a 'difficult' polynomial, namely

$$z^5 - 3z^4 - (2 + i)z^3 + (12 + 5i)z^2 - (8 + 8i)z + 4i.$$

Our method gave the zeros as:

$$\begin{aligned} &0.098684113\bar{5} + 0.455089860\bar{6} i (10), \\ &1.000000000 + 0.000000000 i (13), \\ &1.99999\bar{7}6457 - 0.000000\bar{7}352 i (22), \\ &2.00000\bar{2}3543 + 0.000000\bar{7}352 i (5), \\ &-2.098684113\bar{5} - 0.455089860\bar{8} i (0). \end{aligned}$$

Note that the repeated zero $2 + 0i$ is only accurate to 6 significant figures, which is all that can be expected with a double zero in working to about 11 decimal places, whatever the method. Note also that the second of the repeated zeros took only 5 iterations (since there are always 3 starting and 2 signing off iterations this is the minimum number unless an exact value is found).

Olver (1952), in a survey of desk machine methods, gave a polynomial of degree 16 with coefficients:

$$2.03253121, \quad 3.4356048, \quad 25.1783048, \quad 37.651096, \\ 128.218748, \quad 66.44768, \quad 345.07256, \quad 378.908, \quad 524.327, \\ 468.88, \quad 443.576, \quad 304.08, \quad 190.68, \quad 89.6, \quad 32.8, \quad 8, \quad 1.$$

Our single-length results were as given in **Table 1**. The first wrong digit (underlined) is obtained by comparison with Olver's (1952) double-length working results. The average number of iterations per zero is 9.5 and the zeros appear in increasing order of magnitude.

The polynomial $z^{20} - 20z^{18} + 170z^{16} - 800z^{14} + 2275z^{12} - 400z^{10} + 4290z^8 - 264z^6 + 825z^4 - 100z^2 + 2$ has zeros of the form $\pm a \pm ib$ and, although our first starting values are designed to locate zeros with

Table 1

$$\begin{aligned} &-0.2935045292 + 0.1434992969 i (17), \quad -0.2935045292 - 0.1434992969 i (5), \\ &-0.2244700578 + 0.4509279583 i (13), \quad -0.2244700578 - 0.4509279583 i (5), \\ &-0.1476237802 + 0.77157201\bar{2} i (15), \quad -0.147623780\bar{3} - 0.77157201\bar{3} i (10), \\ &-0.09003999\bar{1}2 + 1.061192059\bar{1} i (12), \quad -0.09003999\bar{2}7 - 1.06119205\bar{8}7 i (8), \\ &-0.0508644\bar{1}89 + 1.296911279\bar{3} i (14), \quad -0.0508644\bar{1}17 - 1.296911280\bar{5} i (7), \\ &-0.0256687598 + 1.474377149\bar{6} i (12), \quad -0.0256687\bar{7}20 - 1.47437714\bar{2}9 i (11), \\ &-0.0104934\bar{8}30 + 1.59629548\bar{3}2 i (10), \quad -0.0104934\bar{7}45 - 1.59629549\bar{7}5 i (6), \\ &-0.0024892\bar{3}46 + 1.66712036\bar{8}3 i (7), \quad -0.0024892\bar{3}66 - 1.66712035\bar{9}8 i (0) \end{aligned}$$

Table 2

$$\begin{array}{l}
-0.499972 - 1.322822 i (43), -0.499976 + 1.322827 i (10), \\
-0.500028 - 1.322929 i (13), -0.500024 + 1.322924 i (10), \\
-0.499947 - 1.322904 i (18), -0.499951 + 1.322899 i (8), \\
-0.500053 - 1.322848 i (9), -0.500048 + 1.322852 i (9), \\
-0.499993 - 1.658240 i (39), -0.499988 + 1.658243 i (8), \\
-0.499928 - 1.658319 i (14), -0.499930 + 1.658324 i (10), \\
-0.500007 - 1.658385 i (12), -0.500012 + 1.658382 i (10), \\
-0.500072 - 1.658306 i (7), -0.500070 + 1.658300 i (0).
\end{array}$$

negative real parts, no more than 19 iterations were required for any zero, the average being 10.9 . The zeros are not stated here but were correct to 10 significant figures on single-length working.

6.2 Double-length arithmetic

The polynomial with factors (z^2+z+1) , $(z^2+z+1.01)$, $(z^2+1.01z+1)$, $(z^2+1.01z+1.01)$ has zeros which form two conjugate 'clusters'. The largest error in a zero found by our method was 28×10^{-15} and the number of iterations for the eight roots were 36, 10, 15, 8, 21, 10, 7 and 0.

An ill-conditioned polynomial given by Olver (1952) and quoted by Wilkinson (1959, p. 168) has coefficients:

1250162561, 385455882, 845947696, 240775148, 247926664, 64249356, 41018752, 9490840, 4178260, 837860, 267232, 44184, 10416, 1288, 224, 16, 2. Our method extracted the roots in the same order as Wilkinson obtained by Bairstow's method; our errors $\times 10^{17}$ were:

$$\begin{array}{rclcl}
& 0 + & 0i, & 0 + & 0i; \\
- & 15 + & 276i, & + & 20 - & 100i; \\
- & 7521 - & 16155i, & - & 4051 + & 5114i; \\
- & 222306 + & 186244i, & - & 290481 - & 56137i;
\end{array}$$

$$\begin{array}{rclcl}
- & 601948 - & 750308i, & - & 267596 + & 221032i; \\
+ & 1050726 + & 1220806i, & + & 456757 - & 353700i; \\
+ & 569153 - & 634862i, & - & 244871 + & 173791i; \\
& 0 + & 10i, & & 0 + & 10i;
\end{array}$$

These errors are at worst $1/200$ of the corresponding errors Wilkinson obtained using a double-length Bairstow method, but our machine worked to approximately two more significant figures.

We conclude this section with a polynomial all of whose zeros are multiple (4th order). Our method, however, located them in a few iterations. The polynomial is $(z^2+z+2)^4(z^2+z+3)^4$ with coefficients 1, 8, 48, 196, 664, 1800, 4198, 8202, 13992, 20228, 25480, 26904, 24385, 17688, 10584, 4320, 1296. Zeros are shown in Table 2.

The correct zeros are $-0.50000000 \pm 1.32287566 i$ and $-0.50000000 \pm 1.65831240 i$. Our answers have, in some cases, errors $O(7 \times 10^{-5})$; this is mostly due to the multiplicity of the zeros, but also to the proximity of the repeated zeros whose imaginary parts have the same sign. Though two of the zeros required about 40 iterations, their conjugates and repeats took much fewer iterations.

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