The use of rational functions in the iterative solution of equations on a digital computer

By P. Jarratt and D. Nudds*

An iterative method for solving a non-linear equation is described, in which a rational function is fitted through previously computed values. Convergence for both single and multiple roots is discussed, first for the case of fitting by linear fractions and then by a more general form.

1. Introduction

The problem of finding solutions along the real axis and in the complex plane of polynomial and transcendental equations in one unknown is of frequent occurrence in scientific and engineering work, and a large number of methods have been described (an extensive bibliography is to be found in Todd, 1962). The advantages and disadvantages of each approach depend on the characteristics of the problem under consideration; generally speaking, however, the methods which are most appropriate for use with a digital computer are those which apply to a wide class of equations and which give rapid convergence.

In this paper we show how rational functions may be used iteratively to find real or complex roots of the nonlinear equation

$$f(z) = 0 \tag{1.1}$$

and we discuss the convergence of the process. The most useful case of linear fractions is considered first and the treatment is then extended to a more general form.

2. Iteration by linear fractions

Suppose that the iteration has been started and that three points $(z_i, f(z_i))$, i = n, n - 1, n - 2, have been found. We choose new coordinates $\xi = z - z_n$ for numerical accuracy, and construct the linear fraction

$$y = \frac{\xi - A}{B\xi + C} \tag{2.1}$$

which passes through the given points. Rearrangement of (2.1) gives

$$\xi = A + B\xi y + Cy \tag{2.2}$$

and we see that A, B and C must satisfy

$$0 = A + Cf_{n}$$

$$\xi_{n-1} = A + B\xi_{n-1}f_{n-1} + Cf_{n-1}$$

$$\xi_{n-2} = A + B\xi_{n-2}f_{n-2} + Cf_{n-2}.$$
(2.3)

The next approximation to the root, ξ_{n+1} , is taken as the zero of (2.1) and hence, solving (2.3) for A, we have

$$\xi_{n+1} = A = \frac{\xi_{n-1} \xi_{n-2} f_n (f_{n-1} - f_{n-2})}{\xi_{n-1} f_{n-1} (f_n - f_{n-2}) + \xi_{n-2} f_{n-2} (f_{n-1} - f_n)}.$$

* Bradford Institute of Technology, Bradford,

In terms of our original coordinates, this becomes

$$-\frac{(z_n-z_{n-1})(z_n-z_{n-2})f_n(f_{n-1}-f_{n-2})}{(z_n-z_{n-2})f_n(f_{n-1}-f_{n-2})}$$

$$+\frac{(z_{n}-z_{n-1})(z_{n}-z_{n-2})f_{n}(f_{n-1}-f_{n-2})}{(z_{n}-z_{n-1})(f_{n-2}-f_{n})f_{n-1}+(z_{n}-z_{n-2})(f_{n}-f_{n-1})f_{n-2}}$$
(2.4)

The iteration is continued by discarding z_{n-2} and repeating the process with the points z_{n+1} , z_n and z_{n-1} . The calculation is terminated when $\left| \frac{z_{n+1} - z_n}{z_n} \right|$ is less than some preassigned number. The situation in which any two function values are equal must be guarded against, as clearly the process given by (2.4) then breaks down. However if, for example, $f_n = f_{n-1}$, then (z_{n-1}, f_{n-1}) may be replaced by (z_{n-1}^*, f_{n-1}^*) , where

$$z_{n-1}^* = \frac{1}{2}(z_n + z_{n-1}),$$

and the iteration continued with the points z_n , z_{n-1}^* , z_{n-2} .

3. Convergence of the method

In order to investigate the convergence of the above process we reformulate (2.2) and (2.3) in terms of the original coordinates to give

$$z = a + bzy + cy$$
,

and
$$z_i = a + bz_iy_i + cy_i$$
, $i = n, n - 1, n - 2$.

For these equations to be consistent we must have

$$\begin{vmatrix} z & zy & y & 1 \\ z_n & z_n y_n & y_n & 1 \\ z_{n-1} & z_{n-1} y_{n-1} & y_{n-1} & 1 \\ z_{n-2} & z_{n-2} y_{n-2} & y_{n-2} & 1 \end{vmatrix} = 0.$$
 (3.1)

Assume a root of (1.1) at $z = \theta$ and define the error ε_i of the *i*th approximation by $\theta = z_i - \varepsilon_i$.

Substituting now in (3.1), recalling that z_{n+1} is found by setting y = 0, and simplifying, we obtain

$$\begin{vmatrix} \varepsilon_{n+1} & 0 & 0 & 1 \\ \varepsilon_n & \varepsilon_n f_n & f_n & 1 \\ \varepsilon_{n-1} & \varepsilon_{n-1} f_{n-1} & f_{n-1} & 1 \\ \varepsilon_{n-2} & \varepsilon_{n-2} f_{n-2} & f_{n-2} & 1 \end{vmatrix} = 0. \quad (3.2)$$

For compactness of notation in the following, we shall denote the determinant of form

$$\begin{vmatrix} \alpha_s & \beta_s & \gamma_s & \dots & \omega_s \\ \alpha_{s-1} & \beta_{s-1} & \gamma_{s-1} & \dots & \omega_{s-1} \\ \vdots & & & & & \\ \alpha_t & \beta_t & \gamma_t & \dots & \omega_t \end{vmatrix}$$

by

$$|\alpha \quad \beta \quad \gamma \quad \ldots \quad \omega |_{s,t}$$

Hence from (3.2) we find

$$\varepsilon_{n+1} = \frac{\left| \varepsilon \quad \varepsilon f \quad f \mid_{n, n-2}}{\left| 1 \quad \varepsilon f \quad f \mid_{n, n-2}}.$$
 (3.3)

Using the expansion of f(z) about the root $z = \theta$, we can write

$$f(z_i) = \sum_{r=1}^{\infty} c_r \epsilon_i^r, \quad i = n, n-1, n-2$$
 (3.4)

where $c_r = \frac{f^{(r)}(\theta)}{r!}$, remembering that $c_0 = f(\theta) = 0$.

Substituting in (3.3) gives

$$\varepsilon_{n+1} = \frac{\left| \begin{array}{ccc} \varepsilon & \sum\limits_{1}^{\infty} c_{r} \varepsilon^{r+1} & \sum\limits_{1}^{\infty} c_{r} \varepsilon^{r} \\ \hline 1 & \sum\limits_{1}^{\infty} c_{r} \varepsilon^{r+1} & \sum\limits_{1}^{\infty} c_{r} \varepsilon^{r} \end{array} \right|_{n,n-2}}{\left| \begin{array}{ccc} 1 & \sum\limits_{1}^{\infty} c_{r} \varepsilon^{r+1} & \sum\limits_{1}^{\infty} c_{r} \varepsilon^{r} \\ \end{array} \right|_{n,n-2}}$$
(3.5)

$$=\frac{\varepsilon_n\varepsilon_{n-1}\varepsilon_{n-2}\left|1\sum_{1}^{\infty}c_r\varepsilon^r\sum_{1}^{\infty}c_r\varepsilon^{r-1}\right|_{n,\,n-2}}{\left|1\sum_{1}^{\infty}c_r\varepsilon^{r+1}\sum_{1}^{\infty}c_r\varepsilon^r\right|_{n,\,n-2}}.$$

Assuming now that the root $z = \theta$ is simple so that $c_1 \neq 0$ and writing $\hat{\varepsilon}_{n, n-2} = \text{Max}\{|\varepsilon_n|, |\varepsilon_{n-1}|, |\varepsilon_{n-2}|\}$ we have

$$1 \sum_{1}^{\infty} c_{r} \varepsilon^{r} \sum_{1}^{\infty} c_{r} \varepsilon^{r-1} \Big|_{n, n-2} = |1 \quad c_{1} \varepsilon \quad c_{3} \varepsilon^{2}|_{n, n-2} + |1 \quad c_{2} \varepsilon^{2} c_{2} \varepsilon|_{n, n-2} + \dots$$
(3.6)

where the remaining terms all have a factor $|1 \varepsilon \varepsilon^2|_{n, n-2}$. Hence (3.6) becomes

$$(c_1c_3-c_2^2)|1 \quad \epsilon \quad \epsilon^2|_{n, n-2}(1+\mathrm{O}(\hat{\epsilon}_{n, n-2})).$$
 (3.7)

Similarly

$$\begin{vmatrix} \mathbf{1} & \sum_{1}^{\infty} c_r \varepsilon^{r+1} & \sum_{1}^{\infty} c_r \varepsilon^r \Big|_{n, n-2} \\ &= |\mathbf{1} & c_1 \varepsilon^2 & c_1 \varepsilon|_{n, n-2} (1 + O(\widehat{\varepsilon}_{n, n-2})). \quad (3.8) \end{aligned}$$

From (3.6), (3.7) and (3.8) we now have

$$\varepsilon_{n+1} = \left(-\frac{c_3}{c_1} + \frac{c_2^2}{c_1^2}\right) \varepsilon_n \varepsilon_{n-1} \varepsilon_{n-2} (1 + \mathcal{O}(\widehat{\varepsilon}_{n, n-2})). \tag{3.9}$$

It is clear from (3.9) that convergence will be assured provided the initial values z_1, z_2, z_3 are sufficiently close to the root. Taking logarithms of both sides of (3.9)

gives

$$\log \varepsilon_{n+1} - \log \varepsilon_n - \log \varepsilon_{n-1} - \log \varepsilon_{n-2}$$

$$= \log K + O(\hat{\varepsilon}_{n, n-2}) \quad (3.10)$$

where $K = -\frac{c_3}{c_1} + \frac{c_2^2}{c_1^2}$. The limiting linear difference equation obtained by neglecting $O(\hat{\varepsilon}_{n, n-2})$ has a solution of the form

$$\log \varepsilon_n = At_1^n + Bt_2^n + Ct_3^n - \frac{1}{2} \log K,$$

where t_1 , t_2 , t_3 are the roots of $t^3 - t^2 - t - 1 = 0$, viz 1.84, $-0.420 \pm 0.606 i$.

As *n* increases, t_2^n and $t_3^n \rightarrow 0$ and hence we can write

$$\varepsilon_n \sim K^{-1/2} R_1^{t_n}, \tag{3.11}$$

where R is a constant depending on the initial approximations chosen. From (3.11) it follows that

$$\varepsilon_{n+1} \sim K^{\frac{t_1-1}{2}} \varepsilon_n^{t_1}. \tag{3.12}$$

Hence the process is of order t_1 or 1.84: after any step in the iteration the increase in the number of accurate significant figures in the modulus of the approximation is 1.84 times the previous increase.

The convergence found using linear fractions is of the same order as that obtained by fitting a quadratic through the latest three points (Muller, 1956). In this case the errors are again related by equation (3.10), but

with
$$K = -\frac{c_3}{c_1}$$
.

However, iteration by linear fractions has a number of general advantages which are discussed in detail in the last section.

4. Convergence at multiple roots

We consider first a double root for which in (3.4) we have $c_1 = 0$, $c_2 \neq 0$. Expanding (3.5) as before, we obtain

$$\varepsilon_{n+1} = \varepsilon_n \varepsilon_{n-1} \varepsilon_{n-2} \frac{c_2 |\mathbf{1} \quad \varepsilon^2 \quad \varepsilon|_{n, n-2} (1 + \mathrm{O}(\widehat{\varepsilon}_{n, n-2}))}{c_2 |\mathbf{1} \quad \varepsilon^3 \quad \varepsilon^2|_{n, n-2} (1 + \mathrm{O}(\widehat{\varepsilon}_{n, n-2}))}.$$

 $|1 \ \epsilon \ \epsilon^2|_{n, n-2}$ is a factor of $|1 \ \epsilon^3 \ \epsilon^2|_{n, n-2}$; extracting this gives

$$\varepsilon_{n+1} = \varepsilon_n \varepsilon_{n-1} \varepsilon_{n-2} \frac{1 + O(\widehat{\varepsilon}_{n, n-2})}{\varepsilon_n \varepsilon_{n-1} + \varepsilon_{n-1} \varepsilon_{n-2} + \varepsilon_{n-2} \varepsilon_n}.$$

The limiting difference equation obtained by neglecting $O(\hat{\varepsilon}_{n, n-2})$ in the above is

$$\frac{1}{\varepsilon_{n+1}} - \frac{1}{\varepsilon_n} - \frac{1}{\varepsilon_{n-1}} - \frac{1}{\varepsilon_{n-2}} = 0. \tag{4.1}$$

This is a linear difference equation in $1/\varepsilon_n$ having the same characteristic roots as (3.10), the equation in $\log \varepsilon_n$ for the case of a simple root. Hence, for large n,

$$\varepsilon_n \sim A/1 \cdot 84^n$$
,

and the convergence is first-order for a double root.

For multiple roots of order p > 2, we have, in (3.4), $c_1 = c_2 = \ldots = c_{p-1} = 0$, $c_p \neq 0$, and (3.5) now gives

$$\varepsilon_{n+1} = \frac{|\varepsilon \quad c_p \varepsilon^{p+1} \quad c_p \varepsilon^p|_{n, n-2} (1 + O(\widehat{\varepsilon}_{n, n-2}))}{|1 \quad c_p \varepsilon^{p+1} \quad c_p \varepsilon^p|_{n, n-2} (1 + O(\widehat{\varepsilon}_{n, n-2}))},$$

or

$$\varepsilon_{n+1} = \varepsilon_n \varepsilon_{n-1} \varepsilon_{n-2} \frac{|1 \quad \varepsilon^p \quad \varepsilon^{p-1}|_{n, n-2}}{|1 \quad \varepsilon^{p+1} \quad \varepsilon^p \quad |_{n, n-2}} (1 + O(\widehat{\varepsilon}_{n, n-2})).$$
(4.2)

The expansion of (4.2) results in a non-linear difference equation in ε_n which has proved intractable. However, it is not difficult to show that there is a solution of the difference equation representing first-order convergence of the form $\varepsilon_n = A/\theta_p^n$, where θ_p is the real root lying between 1 and 2 of the equation

$$x^{p+1} - x^2 - x - 1 = 0.$$

Moreover, this form of convergence has been observed numerically in all the practical cases we have examined.

It is worth noting that, for multiple roots, convergence may be appreciably accelerated by use of Aitken's δ^2 process. Care, however, must be taken that it is not applied too often and, in fact, the process should be used only after the guess found by the previous δ^2 has been discarded.

5. Generalization of the method

We consider now a generalization of the method where we fit a rational function of the form

$$y = \frac{z - a}{b_m z^m + b_{m-1} z^{m-1} + b_{m-2} z^{m-2} + \dots + b_1 z + b_0}$$
(5.1)

through the latest m + 2 points

$$(z_i, f(z_i)), i = n, n-1, \ldots n-m-1.$$

For consistency we require

Again we assume a root at $z = \theta$ and define $z_i = \varepsilon_i + \theta$. By substituting in (5.2) and setting y = 0 to predict the root we obtain after simplification:

and from (5.3) we find

$$\varepsilon_{n+1} = \frac{|\varepsilon \quad f \quad \varepsilon f \dots \varepsilon^m f|_{n, n-m-1}}{|1 \quad f \quad \varepsilon f \dots \varepsilon^m f|_{n, n-m-1}}.$$
 (5.4)

Expanding f(z) about the root $z = \theta$ as in (3.4) and substituting in (5.4) gives

$$\varepsilon_{n+1} = \frac{\left| \frac{\varepsilon \sum_{1}^{\infty} c_r \varepsilon^r \sum_{1}^{\infty} c_r \varepsilon^{r+1} \dots \sum_{1}^{\infty} c_r \varepsilon^{r+m} \right|_{n, n-m-1}}{1 \sum_{1}^{\infty} c_r \varepsilon^r \sum_{1}^{\infty} c_r \varepsilon^{r+1} \dots \sum_{1}^{\infty} c_r \varepsilon^{r+m} \right|_{n, n-m-1}}$$
(5.5)

$$= \varepsilon_n \varepsilon_{n-1} \dots \varepsilon_{n-m-1}$$

$$\times \frac{\left| \begin{array}{cccc} 1 & \sum\limits_{1}^{\infty} c_{r} \varepsilon^{r-1} & \sum\limits_{1}^{\infty} c_{r} \varepsilon^{r} & \ldots & \sum\limits_{1}^{\infty} c_{r} \varepsilon^{r+m-1} \\ \\ 1 & \sum\limits_{1}^{\infty} c_{r} \varepsilon^{r} & \sum\limits_{1}^{\infty} c_{r} \varepsilon^{r+1} & \ldots & \sum\limits_{1}^{\infty} c_{r} \varepsilon^{r+m} \\ \end{array} \right|_{n, \ n-m-1}$$

$$= \varepsilon_n \varepsilon_{n-1} \dots \varepsilon_{n-m-1} (A + O(\widehat{\varepsilon}_{n, n-m-1})),$$

since the lowest-order term in the expansion of each of the determinants contains the alternant

$$|1 \ \varepsilon \ \varepsilon^2 \ldots \varepsilon^{m+1}|_{n, n-m-1},$$

provided $c_1 \neq 0$. A is a constant depending on the values of the constants $c_1, c_2 \dots c_{m+2}$. The resulting difference equation,

$$\log \varepsilon_{n+1} - \sum_{i=n-m-1}^{n} \log \varepsilon_{i} = \log A + O(\widehat{\varepsilon}_{n}, _{n-m-1}),$$

is discussed by Muller (1956). For large n,

$$\varepsilon_n \sim A^{-\frac{1}{n+1}} r^{t_m^n}$$

where again r is arbitrary and t_m , the order of convergence, is the root between 1 and 2 of

$$t^{m+2} = t^{m+1} + t^m + t^{m-1} + \ldots + t + 1.$$

As m increases, $t_m \rightarrow 2$. The first few values are

 $t_0 = 1.62$ (the regula falsi method using the latest two estimates)

 $t_1 = 1.84$ (iteration by linear fractions)

 $t_2 = 1.93$

 $t_3 = 1.97$

 $t_4 = 1.98.$

It is seen that little is gained in speed of convergence by taking m much larger than 1.

For a double root, following the method of Section 4, we obtain from (5.5),

$$\varepsilon_{n+1} = \varepsilon_n \varepsilon_{n-1} \dots \varepsilon_{n-m-1}$$

$$\times \frac{|1 \quad c_2 \varepsilon \quad c_2 \varepsilon^2 \dots c_2 \varepsilon^{m+2}|_{n, n-m-1}}{|1 \quad c_2 \varepsilon^2 \quad c_2 \varepsilon^3 \dots c_2 \varepsilon^{m+3}|_{n, n-m-1}} (1 + O(\widehat{\varepsilon}_{n, n-m-1}))$$

$$= \varepsilon_n \varepsilon_{n-1} \dots \varepsilon_{n-m-1} \times \frac{1}{\sum_{r=n-m-1}^{n} \varepsilon_n \varepsilon_{n-1} \dots \varepsilon_{n-m-1}} (1 + O(\widehat{\varepsilon}_{n, n-m-1})).$$

Neglecting $O(\hat{\varepsilon}_{n, n-m-1})$ gives the linear difference equation in $1/\varepsilon_n$

$$\frac{1}{\varepsilon_{n+1}} = \frac{1}{\varepsilon_n} + \frac{1}{\varepsilon_{n-1}} + \ldots + \frac{1}{\varepsilon_{n-m-1}},$$

so we see that again we have first-order convergence with convergence ratio $1/t_m$.

6. Usefulness of the method

In the comparison of iterative methods for the solution of non-linear equations, an appropriate criterion is the amount of additional accuracy gained at the expense of each additional function evaluation. When the evaluation of derivatives is also necessary this too must be taken into account. Except in special cases where the amount of work involved in evaluating derivatives is much less than that in evaluating the function, the efficiency index (Ostrowski, 1960) is a convenient measure; if a total of m evaluations of the function and its derivatives is needed for each step of the iteration, the efficiency index is equal to the mth root of the order.

Thus, in the Newton-Raphson process, the efficiency index is $\sqrt{2}$. Steffensen's method (Steffensen, 1933), requiring two function evaluations per step, has the same efficiency index. Wegstein's method (Wegstein, 1958), like the regula falsi method using the latest two estimates, has an efficiency index of 1.62. Muller's method and the linear-fractions process present an increased efficiency index of 1.84. For simple roots, the linear-fraction method possesses two important advantages over Muller's method:

(i) there is a saving in time of evaluation of the iterates because of the simpler formula;

 (ii) real roots are found without using complex arithmetic, whereas, in the search for real roots, Muller's method frequently predicts complex approximations.

In addition, the use of linear fractions is advantageous if a root is sought near a simple pole, since in practice other methods often fail completely.

In the case of double roots, Muller's method has the advantage of an efficiency index of $1\cdot 23$. However, the advantages listed above for linear-fractions iteration still apply, and the first-order convergence is easily accelerated by Aitken's δ^2 process. With roots of higher multiplicity, convergence has always resulted for both methods in the cases which we have examined, the first-order convergence of the linear-fractions method invariably being the more rapid.

We have seen that increasing the number of interpolating points improves the efficiency index of the rational-fractions method. The efficiency index improves in the same way for the generalized Muller method of fitting by a higher-degree polynomial, and also for fitting by a completely general rational function (Tornheim, 1964).

But the process is one of diminishing returns, and only if the function evaluation time were overwhelmingly predominant would it be worthwhile to spend extra time in the evaluation of a more complicated iteration formula at each step. In such cases, higher-order methods are only practicable in the rational-function method of the type examined. Muller's generalization presents serious practical difficulties in the location of the appropriate root of the interpolating polynomial. The same strictures apply to the higher-order methods using rational functions in which the numerator is a polynomial of degree higher than unity. For cases where higher-order methods are desirable, one possible approach would be to increase the number of interpolating points at each step of the interpolation, leading to an efficiency index of 2.

References

Muller, D. E. (1956). "Solving Algebraic Equations using an Automatic Computer," M.T.A.C., Vol. 10, p. 208. Ostrowski, A. M. (1960). Solution of Equations and Systems of Equations, New York and London: Academic Press, p. 20. Steffensen, J. F. (1933). "Remarks on Iteration," Skand. Aktuar. Tidskr., Vol. 16, p. 64. Todd, J. (1962). Ed. A Survey of Numerical Analysis, New York: McGraw-Hill. Tornheim, L. (1964). "Convergence of Multipoint Iterative Methods," J. Assoc. Comp. Mach., Vol. 11, p. 210. Wegstein, J. H. (1958). "Accelerating Convergence of Iterative Processes," Comm. Assoc. Comput. Mach., Vol. 1, No. 6, p. 9.