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Note

A Modified Muller Routine for Finding the Zeroes of a Non-analytic Complex Function

A simple modification to the Muller zero-finding routine for complex functions is described which allows the finding of zeroes of complex non-analytic functions. This is particularly useful for the problem of finding all the images produced by a complicated gravitational lens configuration as described here, where it is important not to miss any of the zeroes.

INTRODUCTION

The problem of finding the zeroes of an analytic function of a complex variable by iterative methods has been well studied in numerical analysis, as can be seen in any standard treatment of the subject (see, e.g., Stoer and Bulirsch [1]). In this paper we consider the problem of finding the zeroes for a function which is not analytic over the region of interest.

This problem arises, for example, in the study of the gravitational lens phenomenon (see, e.g., Dyer and Roeder [2]), where one desires to know the location of all possible images produced by the lensing system of a distant source of radiation. If we consider a distant light source (say a quasar), at a distance s_e from a lensing system (say a cluster of spherical galaxies), itself at a distance s_0 from the observer, then the images seen by the observer are located (in a complex plane attached to the sky) at the zeroes of the function $H(z)$:

$$H(z) = z - d - D \sum_{n=1}^{N} \frac{m_n \tilde{f}_n(|z - L_n|)}{(z - L_n)^*},$$

where N is the number of spherical lenses (say galaxies) in the lens system, d gives the location of the undeviated position of the source on the sky, and $D = 4s_0 s_e/(s_0 + s_e)$. Each spherical lens is described by its total mass M_n, its location on the sky L_n, and a density profile function from which the function $\tilde{f}_n(r)$, representing the fractional mass enclosed by a cylinder of radius r, can be derived. Each such mass distribution has a characteristic length scale a, in terms of which all other lengths are measured. For the case of the King mass distribution [3], this function has the form

$$\tilde{f}(k) = \frac{\sqrt{c^2+1}\,\{ln(\sqrt{k^2+1}\,(c+\sqrt{c^2+1})) - \ln(\sqrt{c^2-k^2}+\sqrt{c^2+1})\} + \sqrt{c^2-k^2} - c}{\sqrt{c^2+1}\,\ln(c+\sqrt{c^2+1}) - c},$$

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where a is called the "core radius" for the model, $k = r/a$, and c is the total radius of the spherical object in units of a.

Failure of Muller's Method

The first attempt at finding all the zeroes of this equation used the usual Muller method (see [1, p. 294]) which fits a quadratic to the function at each iteration and then finds the nearest zero of this quadratic, iterating until sufficient accuracy is obtained. When finding multiple zeroes, previously found zeroes are divided out in the usual way. This method was found to be inadequate in that it failed to find all the zeroes that one knew existed in those cases, where symmetry allows prediction of the total number of images. As well, the particular images found depended upon the starting point for Muller's routine. Another disadvantage was the large number of iterations that were required to find many of the zeroes found.

If we take U and V to be the real and imaginary parts, respectively, of $H(z)$, then it can be shown that $U_y + V_x = 0$ and $U_x - V_y = 2(1 - \pi D\sigma)$, where $\sigma(z)$ is the projected mass density on the sky due to all the lensing objects. Hence the Cauchy–Riemann conditions fail except where $\pi D\sigma = 1$. If the Cauchy–Riemann functions are $U_y + V_x = P$ and $U_x - V_y = Q$ then a rotation through an angle $\cos^{-1}(P + Q)/\sqrt{2(P^2 + S^2)}$ will make $U_y + V_x = U_x - V_y = R$, where $R = \sqrt{(P^2 + Q^2)/2}$ is the root-mean-square of P and Q. Hence the difference in magnitude of P and Q is unimportant since it can be transformed away.

Noting that $H(z)$ fails the Cauchy–Riemann conditions, it appeared useful to consider the implications of this for the usual Muller method. Since this method fits the function by a polynomial, it implicitly assumes that the function is itself complex analytic. That this is really the case can be seen by considering the zeroes of a cubic polynomial. Muller's method very quickly finds correctly the zeroes of this function, but when used to find the zeroes of the conjugate function, which fails the Cauchy–Riemann conditions, Muller's method fails.

Having found that Muller's method behaves quite differently when the Cauchy–Riemann conditions fail, we are led to consider the geometry of the two surfaces $U(x, y)$ and $V(x, y)$ over the x–y plane. To find a zero we must, at least implicitly, know the derivatives U_x, U_y, V_x, and V_y. At each iteration we could determine any two of these and then determine the other two from the Cauchy–Riemann equations, enabling us to find the next iteration point. Since Muller's method fits the function in question by a quadratic function, which of course is analytic, these Cauchy–Riemann conditions are assumed, at least implicitly, to be true. To be specific, suppose that U_x and U_y are the two derivatives determined at a point for a function whose conjugate is analytic, so that assuming the validity of the Cauchy–Riemann conditions would yield values for V_x and V_y that are in error by a factor of -1. It is clear that such an error in detecting the correct geometry of the surfaces defined by $U(x, y)$ and $V(x, y)$ will lead to serious problems in finding the zeroes of U and V, as evidenced by the example of the cubic function mentioned above. Clearly, in this simple case the correct choice of the representation of the function is of fundamental importance. In the case of a function like our $H(z)$ the choice of the function or its conjugate is not so simple for it clearly depends on the functions P and Q. Hence, one would like to be able to determine at each iteration which form of the function is the better choice to use in the next Muller iteration.

A Modified Muller's Method

It would appear that there are various methods of determining the choice of the function or its conjugate at each point, such as evaluating the Cauchy–Riemann functions for each case and choosing the representation with the minimum values for these functions. The method we have used appears to be the simplest in terms of programming and only involves one extra function evaluation per iteration. At each iteration two quadratics are fit, one to the function itself and one to the conjugate function. This clearly does not cost a new function evaluation, but only the overhead of the second fit, which is small. Each quadratic is solved for its nearest zero, in each case exactly as in the standard Muller routine. The function is then evaluated at each of these two conditional points. The accepted iteration step is the one of these two yielding the minimum value for the modulus of the function, presumably leading towards a zero. The function evaluation at the accepted iteration point is used in the next iteration while the function evaluation at the rejected point is now redundant. Hence, this requires only one extra function per iteration and requires only minor modification of the standard Muller routine.

This routine has been coded and includes deflation by division for previously found zeroes. As a zero is approached more closely, deflation by very distant previously found zeroes is suppressed to maintain numerical accuracy, in the usual way.

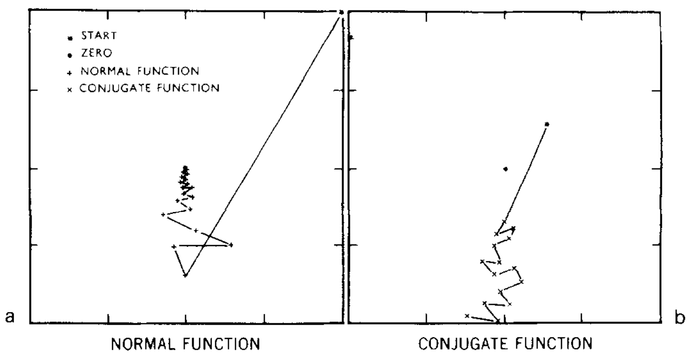

FIG. 1. Successive steps towards a zero of $H(z)$ using Muller's method on the function itself (a), and on the conjugate function (b). In (b) the scale has been changed by a factor of 3.6 to show a larger region.

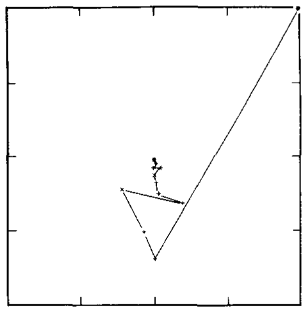

FIG. 2. Successive steps towards the same zero of $H(z)$ using the modified Muller's method, where toggling between function representations is enabled.

The above routine has been used extensively for the multi-image gravitational lens problem described above with great success. In general it uses fewer function evaluations to find *a* given zero, and, much more importantly, it seems able to find all the zeroes in those cases, where we can, by symmetry, predict the total number of zeroes. Thus in this property it seems to continue the well-known property of the usual Muller method, which is exhaustive in finding zeroes of an analytic function.

To illustrate graphically that the standard Muller routine can be enhanced effectively in this way, we have plotted successive iteration steps towards a typical zero using both methods. Fig. 1a shows the usual Muller routine applied to the function itself while Fig. 1b is the result of using the conjugate function. Fig. 2 is the result of using the modified Muller routine, allowing the routine to toggle between the function and its conjugate as it senses the better representation. It is clear in this example that though the zero is eventually reached in Fig. 1a, the successive iteration steps are often close to being perpendicular to the correct direction, while in Fig. 1b (where the scale has changed by a factor of 3.6), the usual Muller routine leads to successive iterations which lose the zero altogether. In contrast, Fig. 2 illustrates the value of letting the routine toggle between representations as necessary, where most steps are taken in roughly the correct direction. It can be seen that the routine does, in fact, change its choice of representation of the function quite frequently, with the function itself the dominant, though not exclusive, choice in the early iterations and changing to the conjugate representation near the zero itself; and hence seems to avoid the large number of steps almost perpendicular to the correct direction.

CONCLUSION

We have described a simple modification to Muller's zero-finding routine which allows one to find all the zeroes of a class of non-analytic complex functions with reasonable efficiency. It has been applied to the gravitational lens problem where the number of zeroes is large (e.g., seventeen, even for only four lenses) and seems to work very well where the conventional Muller routine failed to find all the zeroes.

References

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