DIVISION OF APPLIED MATHEMATICS AND MECHANICS
DEPARTMENT OF ENGINEERING SCIENCES
SCHOOL OF ENGINEERING, UNIVERSITY OF PATRAS

TECHNICAL REPORT No. TR-1984-Y154, 10 September 1984[1]

A new approach to the derivation of exact integral formulae for zeros of analytic functions

Nikolaos I. Ioakimidis

Division of Applied Mathematics and Mechanics, Department of Engineering Sciences, School of Engineering, University of Patras, GR-265 04 Patras, Greece
e-mail: n.ioakimidis@upatras.gr

Abstract A new method for the reduction of the problem of locating the zeros of an analytic function inside a simple closed contour to that of locating the zeros of a polynomial is proposed. The new method (exactly like the presently used classical relevant method) permits in this way the derivation of exact integral formulae for these zeros if they are no more than four. The present approach is based on the solution of a simple homogeneous Riemann–Hilbert boundary value problem. An application to a classical problem in physics concerning neutron moderation is also made and numerical results obtained by using the trapezoidal quadrature rule are presented.

Keywords Complex variables · Analytic functions · Argument principle · Transcendental functions · Zeros · Roots · Exact integral formulae · Closed contours · Riemann–Hilbert boundary value problem · Numerical integration · Trapezoidal quadrature rule · Neutron moderation

1. Introduction

Consider an analytic function $f(z)$ inside and on a simple closed contour C and the classical problem of determination of its zeros a_i in the open bounded region D surrounded by C under the assumption that no zeros of $f(z)$ lie on C. Denote the number of these zeros by n obviously assuming that $n > 0$. Then it is well known that [6]

$$f(z) = \phi(z)\prod_{i=1}^{n}(z-a_i), \quad z \in D, \tag{1}$$

where $\phi(z)$ is also an analytic but non-vanishing function in D and on C. From Eq. (1) it is readily obtained [6]

$$\frac{f'(z)}{f(z)} = \frac{\phi'(z)}{\phi(z)} + \sum_{i=1}^{n}\frac{1}{z-a_i}, \quad z \in D, \quad z \neq a_i, \quad i = 1,2,\ldots,n. \tag{2}$$

[1] Both the internal and the external links (all appearing in blue) were added by the author on 14 January 2018 for the online publication of this technical report.

Now, since $\phi(z)$ does not have zeros in D and on C, we obtain directly from Eq. (2) for the number n of zeros of $f(z)$ in D

$$n = \frac{1}{2\pi i} \oint_C \frac{f'(t)}{f(t)} \mathrm{d}t. \tag{3}$$

Moreover, multiplying both sides of Eq. (2) by z^k, we find in a similar manner that

$$\sum_{i=1}^{n} a_i^k = \frac{1}{2\pi i} \oint_C t^k \frac{f'(t)}{f(t)} \mathrm{d}t, \quad k = 1, 2, \ldots, n. \tag{4}$$

These equations could also have been obtained in a more direct, but equivalent, manner by application of the Cauchy residue theorem to their right-hand sides [6].

After the determination of n from Eq. (3) (or, preferably, in order to avoid the integration in (3), from the argument principle [5]), Eqs. (4) permit the construction of the polynomial

$$p_n(z) = \prod_{i=1}^{n} (z - a_i) \tag{5}$$

with its zeros coinciding with the zeros of $f(z)$ in D on the basis of the well-known Newton identities [6]. For $n \leq 4$ closed-form formulae for these zeros can be derived in an elementary way. For example, for $n = 1$ we have

$$a_1 = \frac{1}{2\pi i} \oint_C t \frac{f'(t)}{f(t)} \mathrm{d}t. \tag{6}$$

The use of this formula was suggested by McCune in 1966 [9]. One year later Delves and Lyness [4] considered the general case of more than one zero of $f(z)$ in D (described also above and in Reference [6]). Numerical results can be obtained by an appropriate application of the trapezoidal quadrature rule [3, 8]. The appearance of the derivative $f'(t)$ of $f(z)$ at $z = t$ in Eqs. (3), (4) and (6) may be disturbing. Delves and Lyness [4] and Carpentier and Dos Santos [2] considered the possibility of deriving equivalent formulae free from the appearance of $f'(t)$ with moderate success. Li [7] also modified this method. It can finally be added that the above method has been successfully used in a long series of problems of physics and engineering for the derivation of closed-form formulae for the zeros of analytic functions and it can be considered today as the classical method for this purpose.

Here we will propose, in Section 2, a related alternative method based also on Eq. (1). An application of this new method to a classical problem in physics will be made in Section 3.

2. The proposed method

Our method consists simply in using Eq. (2) as it stands and its first $n - 1$ derivatives

$$\left[\frac{f'(z)}{f(z)}\right]^{(k-1)} = \left[\frac{\phi'(z)}{\phi(z)}\right]^{(k-1)} - (k-1)! \sum_{i=1}^{n} \frac{1}{(a_i - z)^k},$$
$$k = 1, 2, \ldots, n, \quad z \in D, \quad z \neq a_i, \quad i = 1, 2, \ldots, n, \tag{7}$$

at a point z_0 of D. Essentially without loss of generality, we assume that $z_0 = 0 \in D$ and $f(0) \neq 0$. Then Eqs. (7) yield

$$\sum_{i=1}^{n} \frac{1}{a_i^k} = \frac{1}{(k-1)!} \left\{ \left[\frac{\phi'(z)}{\phi(z)}\right]_{z=0}^{(k-1)} - \left[\frac{f'(z)}{f(z)}\right]_{z=0}^{(k-1)} \right\}, \quad k = 1, 2, \ldots, n. \tag{8}$$

These formulae are analogous to Eqs. (4), but for the reciprocals $1/a_i$ of the zeros a_i of $f(z)$. The Newton identities can further be used for the determination of the polynomial

$$q_n(z) = \prod_{i=1}^{n} (z - 1/a_i) \tag{9}$$

with zeros these numbers, $1/a_i$, exactly as previously.

Taking into account the Cauchy integral formula and the formulae derived by differentiation of this formula [5]

$$f^{(j)}(z) = \frac{j!}{2\pi i} \oint_C \frac{f(t)}{(t-z)^{j+1}} \, \mathrm{d}t, \quad j = 0, 1, \ldots, \tag{10}$$

we find for $z = 0$

$$f^{(j)}(0) = \frac{j!}{2\pi i} \oint_C t^{-j-1} f(t) \, \mathrm{d}t, \quad j = 0, 1, \ldots, n, \tag{11}$$

for $f(z)$ and its first n derivatives required in the second term of the right-hand side of Eqs. (8). From Eqs. (11) we observe that these derivatives were directly expressed in terms of the values $f(t)$ of $f(z)$ along C only.

Now, as far as the first term in the right-hand side of Eqs. (8) is concerned, it is quite easily found from the solution of the elementary Riemann–Hilbert boundary value problem on C

$$\Phi^+(t) = f(t)\, \Phi^-(t) \tag{12}$$

that [1, 5]

$$\Phi^+(z) \equiv f(z) = p_n(z) \exp[\Gamma(z)], \tag{13}$$

$$\Phi^-(z) \equiv 1 = z^{-n} p_n(z) \exp[\Gamma(z)] \tag{14}$$

with $p_n(z)$ defined by Eq. (5) and

$$\Gamma(z) = \frac{1}{2\pi i} \oint_C \frac{\log[t^{-n} f(t)]}{t - z} \, \mathrm{d}t. \tag{15}$$

By comparing Eqs. (1) and (13), we observe (because of Eq. (5)) that

$$\phi(z) = \exp[\Gamma(z)]. \tag{16}$$

Then

$$\frac{\phi'(z)}{\phi(z)} = \Gamma'(z) \tag{17}$$

and because of Eqs. (15) and (17) Eqs. (8) take the simpler equivalent form

$$\sum_{i=1}^{n} \frac{1}{a_i^k} = \frac{k}{2\pi i} \oint_C t^{-k-1} \log[t^{-n} f(t)] \, \mathrm{d}t - \frac{g^{(k-1)}(0)}{(k-1)!}, \quad k = 1, 2, \ldots, n, \tag{18}$$

with

$$g(z) = \frac{f'(z)}{f(z)}. \tag{19}$$

By taking also into account Eqs. (11), we directly observe that the availability of the values $f(t)$ of $f(z)$ on C only is sufficient for the implementation of the present approach and no derivatives of $f(z)$ on C are required.

Finally, we notice that generalizations of the present approach to more complicated cases, like the cases of multiply-connected domains D or infinite domains D (outside the contour C), can be made very easily.

3. An application

As an application, let us now consider the special case of a real function $f(x)$ with only one real zero a_0 and no complex zeros in a circular region D with radius ρ. In this case, obviously, $n=1$ and Eqs. (18) reduce to a single equation, which has the form

$$\frac{1}{a_0}=\frac{1}{2\pi i}\oint_C t^{-2}\log\frac{f(t)}{t}\,\mathrm{d}t-\frac{f'(0)}{f(0)}\,. \tag{20}$$

Putting

$$t=\rho\exp(i\theta)\quad\text{and}\quad\frac{f(t)}{t}=R(\theta)+iI(\theta), \tag{21}$$

we further obtain from Eq. (20)

$$\frac{1}{a_0}=\frac{1}{2\pi\rho}\int_0^{\pi}\left\{\cos\theta\,\log\left[R^2(\theta)+I^2(\theta)\right]+2\sin\theta\,\tan^{-1}\frac{I(\theta)}{R(\theta)}\right\}\mathrm{d}\theta-\frac{f'(0)}{f(0)} \tag{22}$$

as can easily be verified. This equation, not containing complex quantities, is very convenient in practical applications.

Now we consider, as an example, the classical transcendental equation

$$f(x)=x\exp x-c\quad\text{with}\quad c=b\exp b, \tag{23}$$

appearing in a problem of neutron moderation in nuclear reactors. This equation was already studied in References [10] and [1]. Moreover, the same equation for $b<-1$ possesses one real zero a_0 in the interval $(-1,0)$. Therefore, we find from Eq. (22) (with $\rho=1$) that

$$\frac{1}{a_0}=\frac{1}{2\pi}\int_0^{\pi}\left\{\cos\theta\,\log\left[R^2(\theta)+I^2(\theta)\right]+2\sin\theta\,\tan^{-1}\frac{I(\theta)}{R(\theta)}\right\}\mathrm{d}\theta+\frac{1}{c}\,, \tag{24}$$

where now

$$R(\theta)=\cos(\sin\theta)\,\exp(\cos\theta)-c\,\cos\theta, \tag{25}$$

$$I(\theta)=\sin(\sin\theta)\,\exp(\cos\theta)+c\,\sin\theta. \tag{26}$$

Two further equations for the determination of a_0, which are somewhat analogous to Eq. (24), were proposed in Reference [1]. Numerical results obtained from Eq. (24) in the cases studied in Reference [1] by using the trapezoidal quadrature rule [3, 8] (exactly as in Reference [1]) with $n=5,10,\ldots,25$ nodes are displayed in Table 1 below for five values of the constant b in the second of Eqs. (23). These numerical results both verify the validity of Eq. (24) together with Eqs. (25) and (26) and, moreover, in all cases, they were found more accurate than the corresponding numerical results displayed in Reference [1].

Table 1. Numerical results for the zero a_0 of Eq. (23) for $b=-1.1$, -1.5, -3, -5 and -10, obtained from Eq. (24) together with Eqs. (25) and (26) by using the trapezoidal quadrature rule with $n=5,10,\ldots,25$ nodes.

n	$b=-1.1$	$b=-1.5$	$b=-3$	$b=-5$	$b=-10$
5	−0.85510767	−0.62473883	−0.17856061	−0.034885768	−0.00045420555
10	−0.89522470	−0.62577600	−0.17856063	−0.034885768	−0.00045420555
15	−0.90333025	−0.62578247	−0.17856063	−0.034885768	−0.00045420555
20	−0.90540656	−0.62578253	−0.17856063	−0.034885768	−0.00045420555
25	−0.90599408	−0.62578253	−0.17856063	−0.034885768	−0.00045420555

4. Conclusions

Concluding, we can add that, in our opinion, closed-form formulae for the zeros of transcendental functions like Eqs. (22) and (24) should be preferable in practice to the direct determination of such a zero by the methods of numerical analysis since they are valid for all values of the parameters in the transcendental function like b in Eq. (23). On the contrary, any numerical determination of such a zero will be useless for different values of the parameters in the transcendental function. On the other hand, these closed-form formulae are also of sufficient theoretical interest both because they are simply closed-form formulae and because of the fact that algebraic manipulations can be performed on these formulae (such as series expansions and differentiations with respect to some parameters). Finally, the present approach seems to be a very simple one and, simultaneously, it leads to derivative-free formulae for the sought zeros.

Acknowledgements The present results were obtained in the course of a research project supported by the Greek General Secretariat of Research and Technology. The author is thankful to this General Secretariat for the financial support of this project.

References

[1] E. G. Anastasselou and N. I. Ioakimidis, A generalization of the Siewert–Burniston method for the determination of zeros of analytic functions, *Journal of Mathematical Physics*, **25** (1984), 2422–2425. https://doi.org/10.1063/1.526448

[2] M. P. Carpentier and A. F. Dos Santos, Solution of equations involving analytic functions, *Journal of Computational Physics*, **45** (1982), 210–220. https://doi.org/10.1016/0021-9991(82)90117-6

[3] P. J. Davis and P. Rabinowitz, *Methods of Numerical Integration*, 2nd Edn. Academic Press, Orlando, FL, 1984, pp. 51–57, 168–172 and 314–316. https://www.sciencedirect.com/science/book/9780122063602. Dover Edn: http://store.doverpublications.com/0486453391.html

[4] L. M. Delves and J. N. Lyness, A numerical method for locating the zeros of an analytic function, *Mathematics of Computation*, **21** (1967), 543–560. https://doi.org/10.2307/2004999

[5] F. D. Gakhov, *Boundary Value Problems*. Pergamon Press, Oxford, and Addison-Wesley, Reading, MA, 1966, pp. 28–29, 85–86 and 92–96. https://www.sciencedirect.com/science/book/9780080100678

[6] A. S. Householder, *The Numerical Treatment of a Single Nonlinear Equation*. McGraw-Hill, New York, NY, 1970, pp. 36–38, 188 and 191–192.

[7] T.-Y. Li, On locating all zeros of an analytic function within a bounded domain by a revised Delves/Lyness method, *SIAM Journal on Numerical Analysis*, **20** (1983), 865–871. https://doi.org/10.1137/0720058

[8] J. N. Lyness and L. M. Delves, On numerical contour integration round a closed contour, *Mathematics of Computation*, **21** (1967), 561–577. https://doi.org/10.2307/2005000

[9] J. E. McCune, Exact inversion of dispersion relations, *Physics of Fluids*, **9** (1966), 2082–2084. https://doi.org/10.1063/1.1761574

[10] C. E. Siewert and A. R. Burkart, An asymptotic solution in the theory of neutron moderation, *Nuclear Science and Engineering*, **54** (1974), 455–456. https://doi.org/10.13182/NSE74-A23440