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algorithm for computing zeros of  
analytic functions**

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*Report TW 339, June 2002*



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## **Abstract**

We consider the quadrature method developed by Kravanja and Van Barel (Computing 63(1):69–91, 1999) for computing all the zeros of an analytic function that lie inside the unit circle. The algorithm uses only the function values and no (first or higher order) derivatives. Information about the location of the zeros is obtained from certain integrals along the unit circle. In numerical computations these are replaced by their trapezoidal rule approximations. We investigate the resulting quadrature error. Our error analysis shows that it actually has no effect at all on the computed approximations for the zeros.

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## Abstract

We consider the quadrature method developed by Kravanja and Van Barel (Computing 63(1):69–91, 1999) for computing all the zeros of an analytic function that lie inside the unit circle. The algorithm uses only the function values and no (first or higher order) derivatives. Information about the location of the zeros is obtained from certain integrals along the unit circle. In numerical computations these are replaced by their trapezoidal rule approximations. We investigate the resulting quadrature error. Our error analysis shows that it actually has no effect at all on the computed approximations for the zeros.

## 1 Introduction

Let  $\mathbb{T}$  denote the unit circle in the complex plane and let  $f$  be analytic inside and on  $\mathbb{T}$ . Assume that  $f$  has no zeros on  $\mathbb{T}$ . We consider the problem of computing *all* the zeros of  $f$  that lie inside  $\mathbb{T}$ .

Our approach can be seen as a continuation of the pioneering work of Delves and Lyness [3].

Let  $N$  denote the total number of zeros of  $f$  that lie inside  $\mathbb{T}$ , i.e., the number of zeros where each zero is counted according to its multiplicity. Suppose from now on that  $N > 0$ . Delves and Lyness considered the sequence  $Z_1, \dots, Z_N$  that consists of all the zeros of  $f$  that lie inside  $\mathbb{T}$ . Each zero is repeated according to its multiplicity. Suppose that the first derivative  $f'$  is available. An easy calculation shows that the logarithmic derivative  $f'/f$  has a simple pole at each zero of  $f$  with residue equal to the multiplicity of

the zero. Cauchy's Theorem implies that

$$N = \frac{1}{2\pi i} \int_{\mathbb{T}} \frac{f'(z)}{f(z)} dz.$$

This formula enables one to calculate  $N$  via numerical integration. Methods for the determination of zeros of analytic functions that are based on the numerical evaluation of integrals are called *quadrature methods*. A review of such methods was given by Ioakimidis [4]. Delves and Lyness considered the integrals

$$s_p := \frac{1}{2\pi i} \int_{\mathbb{T}} z^p \frac{f'(z)}{f(z)} dz, \quad p = 0, 1, 2, \dots$$

The residue theorem implies that the  $s_p$ 's are equal to the *Newton sums* of the unknown zeros,

$$s_p = Z_1^p + \dots + Z_N^p, \quad p = 0, 1, 2, \dots$$

These  $s_p$ 's can be calculated via numerical integration along the unit circle.

Delves and Lyness considered the monic polynomial of degree  $N$  that has zeros  $Z_1, \dots, Z_N$ ,

$$P_N(z) := \prod_{k=1}^N (z - Z_k). \tag{1}$$

This polynomial is called the *associated polynomial* for the interior of  $\mathbb{T}$ . Its coefficients in the standard monomial basis can be calculated from the Newton sums via Newton's identities. In this way Delves and Lyness reduced the problem to the easier problem of computing the zeros of a polynomial. Unfortunately, the map from the Newton sums to the coefficients of  $P_N$  in the standard monomial basis is usually ill-conditioned. Also, the polynomials that arise in practice may be such that small changes in the coefficients produce much larger changes in some of the zeros. This ill-conditioning of the map between the coefficients of a polynomial and its zeros was investigated by Wilkinson [14]. The location of the zeros determines their sensitivity to perturbations of the coefficients. Multiple zeros and very close zeros are very sensitive, but even a succession of moderately close zeros can result in severe ill-conditioning. Wilkinson stated that ill-conditioning in polynomials cannot be overcome without, at some stage of the computation, resorting to high precision arithmetic.

If  $f$  has many zeros inside  $\mathbb{T}$ , then the associated polynomial is of high degree and could be very ill-conditioned. Therefore, if  $N$  is large, one has to calculate its coefficients and thus the integrals  $s_1, \dots, s_N$  very accurately. To avoid the use of high precision arithmetic and to reduce the number of integrand evaluations needed to approximate the  $s_p$ 's, Delves and Lyness suggested to construct and solve the associated polynomial only if its degree is smaller than or equal to a preassigned number. Otherwise, the interior of  $\mathbb{T}$  is subdivided or covered with a finite covering and the smaller regions are treated in turn.

For decades, the method of Delves and Lyness was the method of choice for computing zeros of analytic functions.

In recent years, we have argued that what is wrong with this approach is that Delves and Lyness considered the wrong set of unknowns, cf. our paper [7] and the book [9]. One should consider the mutually distinct zeros and their respective multiplicities *separately*. The new quadrature method that we have presented is a generalization of the method of Delves and Lyness. It is again based on the numerical evaluation of integrals along  $\mathbb{T}$  that involve the logarithmic derivative  $f'/f$ , but by using the theory of formal orthogonal polynomials we have been able to obtain more accurate approximations for the zeros. The Fortran 90 package ZEAL [10] contains an implementation of our algorithm. In this approach, the mutually distinct zeros are computed by solving a generalized eigenvalue problem whereas the multiplicities are calculated by solving a linear system of equations that has Vandermonde structure. The number of mutually distinct zeros is determined indirectly. Our method is self-starting in the sense that it does not require initial approximations of the zeros.

In some applications, the calculation of the derivative  $f'$  is more time-consuming than that of  $f$ . Delves and Lyness used an integration by parts to derive a formula for  $s_p$  that depends only on a multi-valued logarithm of  $f$  and not on  $f'$ . To apply this formula, they had to keep track of the sheet on which  $\log f(z)$  lies as  $z$  runs along  $\mathbb{T}$ . Unfortunately, in most cases it is impossible to do this in a completely reliable way, i.e., without accidentally overlooking any sheets. Carpentier and Dos Santos [1] and Davies [2] derived similar formulae. See also Ioakimidis and Anastasselou [5].

The approach that we took in [7] involves integrals along the unit circle that contain the logarithmic derivative  $f'/f$ . In [8] we have shown that essentially the same results can be obtained via integrals that contain  $1/f$ .

The derivative  $f'$  is no longer needed. Of course, in this approach not the mutually distinct zeros but rather the unknowns  $Z_1, \dots, Z_N$  are calculated and the multiplicities cannot be computed explicitly. But apart from this, the algorithm has the same advantages as the algorithm in [7]. In particular, it does not require initial approximations for the zeros and we have found that it gives accurate results. The value of  $N$  is computed via the principle of the argument, or, equivalently, as a winding number. For a discussion of various reliability issues concerning this calculation, we refer to [8].

The integrals along the unit circle that appear in our approach are to be evaluated via numerical integration. Until recently, we have been silent about the influence of the inevitable integration error upon the quality of the computed approximations for the zeros of  $f$  that lie inside  $\mathbb{T}$ . However, for our approach involving both  $f$  and  $f'$ , in [6, 11] we have been able to prove that the integration error has no influence at all in case the trapezoidal rule is used. This quadrature rule was already recommended since, when written as Riemann integrals, the integrals involve periodic functions over a complete period.

In this paper we will show that a similar result holds for our algorithm that does not rely on the derivative  $f'$ . However, the techniques used in our previous error analysis are no longer applicable, which is why we present our results in a separate publication. Also, our proof relies on a splitting of  $1/f$  that is likely to be useful in other settings as well, notably for factoring algorithms (see, e.g., [12, 13]).

## 2 Error analysis

Let  $\mathcal{P}$  be the linear space of polynomials with complex coefficients. One defines a symmetric bilinear form

$$\langle \cdot, \cdot \rangle_\star : \mathcal{P} \times \mathcal{P} \rightarrow \mathbb{C}$$

by setting

$$\langle \phi, \psi \rangle_\star := \frac{1}{2\pi i} \int_{\mathbb{T}} \phi(z) \psi(z) \frac{1}{f(z)} dz$$

for any two polynomials  $\phi, \psi \in \mathcal{P}$ .

Let us write  $f$  as  $f = P_N g$  where  $P_N$  is as in (1) and where the function  $g$  is analytic inside and on  $T$  and has no zeros in this region.

Define  $g_{N-1}(z)$  as the polynomial of degree  $N - 1$  that interpolates  $1/g$  at the zeros of  $f$  in the sense of Hermite:

$$g_{N-1}^{(l)}(z_k) = \left(\frac{1}{g}\right)^{(l)}(z_k), \quad k = 1, \dots, n, \quad l = 0, 1, \dots, \nu_k - 1$$

where  $n$  denotes the number of mutually distinct zeros of  $f$  that lie inside  $\mathbb{T}$ ,  $z_1, \dots, z_n$  denote these zeros, and  $\nu_1, \dots, \nu_n$  their respective multiplicities.

Then we can write  $1/f$  as

$$\frac{1}{f} = \frac{1}{P_N g} = \frac{g_{N-1}}{P_N} + \frac{h}{g}$$

where the function  $h$  is defined by

$$h := \frac{1 - g_{N-1}g}{P_N}.$$

One can easily verify that  $h$  is analytic inside and on  $\mathbb{T}$ . It follows that

$$\langle \phi, \psi \rangle_\star = \frac{1}{2\pi i} \int_{\mathbb{T}} \phi(z) \psi(z) \frac{g_{N-1}(z)}{P_N(z)} dz$$

for any two polynomials  $\phi, \psi \in \mathcal{P}$ .

The residue theorem now immediately implies that

$$\langle z^p, P_N(z) \rangle_\star = 0, \quad p = 0, 1, 2, \dots$$

This equation is to be interpreted in two steps.

First, it implies that  $P_N$  is “orthogonal” to all polynomials of lower degree. In [8] it is shown that  $P_N$  is actually the *only* monic polynomial of degree  $N$  having this property, which identifies  $P_N$  as the *regular formal orthogonal polynomial* (FOP) of degree  $N$  (for a definition, we refer to [8]) and leads to a computational procedure for calculating its zeros that involves a generalized eigenvalue problem. These zeros of  $P_N$  coincide with the zeros of  $f$  that we are looking for.

Second,  $P_N$  is also orthogonal to *all* polynomials of degree  $N$  or higher. In [8] we have proved that  $P_N$  is actually the last regular FOP, i.e., there exists no regular FOP of degree larger than  $N$ , a result which then leads to a stopping criterion in the final version of the algorithm.

We will now investigate the quadrature error. Let

$$\omega_l := \exp\left(\frac{2\pi i}{K}l\right), \quad l = 0, 1, \dots, K-1,$$

be the  $K$ th roots of unity. Then the  $K$ -point trapezoidal rule approximation for  $\langle \phi, \psi \rangle_\star$  is given by

$$\langle \phi, \psi \rangle_\star^{(K)} := \frac{1}{K} \sum_{l=0}^{K-1} \phi(\omega_l) \psi(\omega_l) \frac{\omega_l g_{N-1}(\omega_l)}{P_N(\omega_l)}.$$

Let  $g_{N-1}(z) =: \gamma_0 + \gamma_1 z + \dots + \gamma_{N-1} z^{N-1}$  and define  $\gamma_j := 0$  for  $j \geq N$ . Assume that  $K > N$ . Then the following holds.

**Theorem 1**  $\langle z^p, P_N(z) \rangle_\star^{(K)} = \gamma_{K-1-p}$  for  $p = 0, 1, \dots, K-1$ .

*Proof.* One can easily verify that

$$\begin{aligned} \langle z^p, P_N(z) \rangle_\star^{(K)} &= \frac{1}{K} \sum_{l=0}^{K-1} \omega_l^{p+1} g_{N-1}(\omega_l) \\ &= \frac{1}{K} \sum_{l=0}^{K-1} \omega_l^{p+1} \sum_{j=0}^{K-1} \gamma_j \omega_l^j \\ &= \frac{1}{K} \sum_{j=0}^{K-1} \gamma_j \sum_{l=0}^{K-1} \omega_l^{p+j+1}. \end{aligned}$$

Since

$$\sum_{l=0}^{K-1} \omega_l^{p+j+1} = \sum_{l=0}^{K-1} \left[ \exp\left(\frac{2\pi i}{K}\right) \right]^{(p+j+1)l}$$

it follows that the sum in the left-hand side is equal to  $K$  if  $p+j+1 = K$  and zero otherwise. (Actually, the sum is equal to  $K$  if  $p+j+1$  is an integer multiple of  $K$  but the fact that  $0 \leq p, j \leq K-1$  implies that  $1 \leq p+j+1 \leq 2K-1$ ; hence, only the case  $p+j+1 = K$  can occur.) We may conclude that

$$\langle z^p, P_N(z) \rangle_\star^{(K)} = \frac{1}{K} \sum_{j=0}^{K-1} \gamma_j (K \delta_{j, K-1-p}) = \gamma_{K-1-p}.$$

This proves the theorem. □

**Corollary 2**  $\langle z^p, P_N(z) \rangle_\star^{(K)} = 0$  for  $p = 0, 1, \dots, K - 1 - N$ .

If we can establish that  $P_N$  is the (unique!) regular formal orthogonal polynomial of degree  $N$  with respect to the symmetric bilinear form  $\langle \cdot, \cdot \rangle_\star^{(K)}$ , then we will have made our point, as this implies that the zeros of  $P_N$ , which are precisely the zeros of  $f$  that we are looking for, can be computed by solving a generalized eigenvalue problem. This generalized eigenvalue problem is the one that is actually solved by the algorithm that we presented in [8] as soon as the trapezoidal rule approximations are used instead of the underlying integrals. If  $P_N$  is the regular formal orthogonal polynomial of degree  $N$  for *both* symmetric bilinear forms, then the results are the same and the quadrature error has no influence at all.

The previous corollary immediately implies that  $P_N$  is a formal orthogonal polynomial with respect to  $\langle \cdot, \cdot \rangle_\star^{(K)}$  if  $K \geq 2N$ . We will need to impose this condition throughout the rest of our analysis.

**Corollary 3** If  $K \geq 2N$ , then  $\langle z^p, P_N(z) \rangle_\star^{(K)} = 0$  for  $p = 0, 1, \dots, N - 1$ .

The uniqueness of  $P_N$  as a monic formal orthogonal polynomial of degree  $N$  for the form  $\langle \cdot, \cdot \rangle_\star$  was established by using its “over-orthogonality”, i.e., the fact that  $P_N$  is also orthogonal to *all* polynomials of degree  $N$  or higher. In the case of the form  $\langle \cdot, \cdot \rangle_\star^{(K)}$  this is no longer true. The property holds up to a certain degree (depending on the value of  $K$ ) but it does not hold for all degrees. We need to proceed differently (and the proof is more complicated).

**Theorem 4** If  $K \geq 2N$ , then  $P_N$  is the only monic polynomial of degree  $N$  that is orthogonal to all polynomials of lower degree with respect to  $\langle \cdot, \cdot \rangle_\star^{(K)}$ .

*Proof.* Suppose that  $Q_N$  is another monic polynomial of degree  $N$  that has the same property. The orthogonality conditions

$$\langle z^p, Q_N(z) \rangle_\star^{(K)} = 0, \quad p = 0, 1, \dots, N - 1,$$

can be written as

$$\frac{1}{K} \sum_{l=0}^{K-1} \omega_l^{p+1} g_{N-1}(\omega_l) \frac{Q_N(\omega_l)}{P_N(\omega_l)} = 0, \quad p = 0, 1, \dots, N - 1.$$

In matrix notation:

$$\begin{bmatrix} \omega_0 & \omega_1 & \cdots & \omega_{K-1} \\ \omega_0^2 & \omega_1^2 & \cdots & \omega_{K-1}^2 \\ \vdots & \vdots & & \vdots \\ \omega_0^N & \omega_1^N & \cdots & \omega_{K-1}^N \end{bmatrix} \begin{bmatrix} g_{N-1}(\omega_0) \frac{Q_N(\omega_0)}{P_N(\omega_0)} \\ \vdots \\ g_{N-1}(\omega_{K-1}) \frac{Q_N(\omega_{K-1})}{P_N(\omega_{K-1})} \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix}.$$

The  $N \times K$  matrix in the left-hand side has (full) rank  $N$ . A basis for its null space is given by the columns of the  $K \times (K - N)$  matrix

$$S := \begin{bmatrix} 1 & \omega_0 & \cdots & \omega_0^{K-N-1} \\ \vdots & \vdots & & \vdots \\ 1 & \omega_{K-1} & \cdots & \omega_{K-1}^{K-N-1} \end{bmatrix}.$$

It follows that there exists (one and only one) vector  $\rho \in \mathbb{C}^{K-N-1}$  such that

$$\left[ g_{N-1}(\omega_l) \frac{Q_N(\omega_l)}{P_N(\omega_l)} \right]_{l=0}^{K-1} = S\rho.$$

Let  $\rho =: [\rho_j]_{j=0}^{K-N-1}$  and  $r_{K-N-1}(z) := \sum_{j=0}^{K-N-1} \rho_j z^j$ . Then

$$g_{N-1}(\omega_l) \frac{Q_N(\omega_l)}{P_N(\omega_l)} = r_{K-N-1}(\omega_l), \quad l = 0, 1, \dots, K-1,$$

or, since  $P_N(\omega_l) \neq 0$  for  $l = 0, 1, \dots, K-1$ ,

$$P_N(\omega_l) r_{K-N-1}(\omega_l) - Q_N(\omega_l) g_{N-1}(\omega_l) = 0, \quad l = 0, 1, \dots, K-1.$$

Since  $\deg(P_N r_{K-N-1} - Q_N g_{N-1}) = \max(N + (K - N - 1), 2N - 1) = K - 1$  and since a polynomial of degree  $K - 1$  is completely determined by its values at  $K$  distinct points, it follows that

$$P_N(z) r_{K-N-1}(z) = Q_N(z) g_{N-1}(z) \tag{2}$$

for every  $z \in \mathbb{C}$ . Thus  $g_{N-1}$  and  $r_{K-N-1}$  are of the same degree and have the same highest degree coefficient. Hence, we can write  $r_{N-1}$  instead of  $r_{K-N-1}$ . As  $g_{N-1}(z_k) = (1/g)(z_k) \neq 0$  for  $k = 1, \dots, n$  it follows that the zeros of  $P_N$ , including multiplicity, all need to go into  $Q_N$  for (2) to hold. Since  $Q_N$  is of degree  $N$ , we may conclude that indeed  $P_N \equiv Q_N$ , and also  $r_{N-1} \equiv g_{N-1}$ . This proves the theorem.  $\square$

### 3 Conclusion

Let us summarize our results by explicitly stating the (Hankel version of the) generalized eigenvalue problems. (In practice, a change of basis is to be

used, which results in another version of these eigenvalue problems. We have studied this extensively in previous publications and it does not concern us here.) Define

$$H_N^* := \left[ \langle z^p, z^q \rangle_\star \right]_{p,q=0}^{N-1} \quad \text{and} \quad H_N^{*\leq} := \left[ \langle z^p, z z^q \rangle_\star \right]_{p,q=0}^{N-1}.$$

The fact that  $P_N$  is the regular FOP of degree  $N$  for  $\langle \cdot, \cdot \rangle_\star$  implies that its zeros, in other words the zeros  $Z_1, \dots, Z_N$  of  $f$  that lie inside the unit circle, are given by the eigenvalues of the pencil  $H_N^{*\leq} - \lambda H_N^*$ . Since  $P_N$  is also the regular FOP for  $\langle \cdot, \cdot \rangle_\star^{(K)}$  if  $K \geq 2N$ , it follows that in this case the eigenvalues of the pencil  $\hat{H}_N^{*\leq} - \lambda \hat{H}_N^*$ , where

$$\hat{H}_N^* := \left[ \langle z^p, z^q \rangle_\star^{(K)} \right]_{p,q=0}^{N-1} \quad \text{and} \quad \hat{H}_N^{*\leq} := \left[ \langle z^p, z z^q \rangle_\star^{(K)} \right]_{p,q=0}^{N-1},$$

are also given by  $Z_1, \dots, Z_N$ . The latter pencil is the one that is used in numerical computations when the integrals along  $\mathbb{T}$  are replaced by their corresponding trapezoidal rule approximations. *Our error analysis shows that if the number of quadrature points used in the trapezoidal rule is larger than or equal to twice the number of zeros of  $f$  that lie inside the unit circle, then the resulting quadrature error has no influence at all on the accuracy of the computed approximations for these zeros.*

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