Available at WWW.MATHEMATICSWEB.ORG
POWERED BY SCIENCE @ DIRECT•

ELSEVIER

Journal of Computational and Applied Mathematics 152 (2003) 467–480

JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS

www.elsevier.com/locate/cam

An error analysis of two related quadrature methods for computing zeros of analytic functions

Tetsuya Sakurai[a,*], Peter Kravanja[b], Hiroshi Sugiura[c], Marc Van Barel[b]

[a] *Institute of Information Sciences and Electronics, University of Tsukuba, Tennodai 1-1-1, Tsukuba, Ibraraki, 305-8573, Japan*
[b] *Katholieke Universiteit Leuven, Department of Computer Science, Celestijnenlaan 200 A, B-3001 Heverlee, Belgium*
[c] *Graduate School of Engineering, Nagoya University, Nagoya 464-8603, Japan*

Received 30 November 2001; received in revised form 22 May 2002

Abstract

We present an error analysis for two related quadrature methods (the Delves–Lyness method and its modification by Kravanja, Sakurai and Van Barel) for computing all the zeros of an analytic function that lie inside the unit circle. We consider the forward as well as the backward approximation error in case the integrals are computed via the trapezoidal rule on the unit circle. Contrary to the Delves–Lyness method, the quadrature error that arises from the zeros located inside the unit circle does not affect the results of the approach of Kravanja et al. Numerical experiments illustrate our main results.

Keywords: Zeros of analytic functions; Error analysis; Quadrature methods

1. Introduction

Let the complex function f be analytic in a simply connected region W of the complex plane that includes the closed unit disk. Assume that f has no zeros on the unit circle $\mathbb{T}$. We consider the problem of computing *all* the zeros of f that lie inside $\mathbb{T}$, together with their respective multiplicities.

Methods for the determination of zeros of analytic functions that are based on the numerical evaluation of integrals are called *quadrature methods* [8]. Our approach to this problem can be seen as a continuation of the pioneering work by Delves and Lyness [4].

* Corresponding author. Tel./fax: +81-298-53-3276.
E-mail addresses: sakurai@is.tsukuba.ac.jp (T. Sakurai), peter.kravanja@na-net.ornl.gov (P. Kravanja), sugiura@nuie.nagoya-u.ac.jp (H. Sugiura), marc.vanbarel@cs.kuleuven.ac.be (M. Van Barel).

PII: S0377-0427(02)00724-0

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 that $N > 0$. The value of N can be calculated via numerical integration or by applying the principle of the argument [6,21]. We may therefore assume that N is known.

Let n denote the number of mutually distinct zeros of f that lie inside $\mathbb{T}$. Let $z_1, \ldots, z_n$ be these zeros and $v_1, \ldots, v_n$ their respective multiplicities.

Define the *associated polynomial* P_N of degree N as

$$P_N(z) := \prod_{k=1}^{n} (z - z_k)^{v_k}.$$

Let the complex function $g: W \to \mathbb{C}$ be defined by $f = P_N g$. Then g is analytic in W and g has no zeros inside and on $\mathbb{T}$. The following holds:

$$\frac{f'(z)}{f(z)} = \frac{P_N'(z)}{P_N(z)} + \frac{g'(z)}{g(z)} = \sum_{k=1}^{n} \frac{v_k}{z - z_k} + \frac{g'(z)}{g(z)}.$$

The second term on the right-hand side, g'/g, is analytic inside and on $\mathbb{T}$. It follows that f'/f is meromorphic inside and on $\mathbb{T}$, with simple poles at the z_k and corresponding residues equal to v_k.

Define the *moments* μ_p as

$$\mu_p := \frac{1}{2\pi i} \int_{\mathbb{T}} z^p \frac{f'(z)}{f(z)} \, \mathrm{d}z, \quad p = 0, 1, 2, \ldots \, .$$

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

$$\mu_p = \sum_{k=1}^{n} v_k z_k^p, \quad p = 0, 1, 2, \ldots \, . \tag{1}$$

Delves and Lyness calculated the coefficients of P_N in the standard monomial basis,

$$P_N(z) =: z^N + \sigma_1 z^{N-1} + \cdots + \sigma_N,$$

via Newton's identities.

Theorem 1 (Newton's identities).

$$\mu_1 + \sigma_1 = 0$$

$$\mu_2 + \mu_1 \sigma_1 + 2\sigma_2 = 0$$

$$\vdots$$

$$\mu_N + \mu_{N-1}\sigma_1 + \cdots + \mu_1 \sigma_{N-1} + N\sigma_N = 0.$$

Proof. An elegant proof was given by Carpentier and Dos Santos [1]. □

In this way, Delves and Lyness reduced the problem to the easier problem of computing the zeros of a polynomial. First, the moments $\mu_1, \ldots, \mu_N$ are approximated via numerical integration along $\mathbb{T}$

and then Newton's identities are used to obtain approximations for the coefficients $\sigma_1, \ldots, \sigma_N$:

$$\sigma_k = -\left(\mu_k + \sum_{j=1}^{k-1} \mu_{k-j}\sigma_j\right)/k, \quad k = 1, 2, \ldots, N. \tag{2}$$

Unfortunately, the map from the Newton sums to the coefficients of P_N is usually ill-conditioned. Also, the associated polynomials that arise in practice may be such that small changes in the coefficients produce much larger changes in some of the zeros.

As some of the authors of the present paper have argued elsewhere, what is wrong with the approach taken by Delves and Lyness is that it considers the wrong set of unknowns. One should consider the mutually distinct zeros and their respective multiplicities *separately*. This is the approach that was proposed by Kravanja et al. [9,14,10,12]. It leads to a quadrature method that generalizes the approach of Delves and Lyness. The mutually distinct zeros are given by the eigenvalues of a generalized eigenvalue problem involving the following *Hankel matrices*:

$$H_n := \begin{bmatrix} \mu_0 & \mu_1 & \cdots & \mu_{n-1} \\ \mu_1 & & \iddots & \vdots \\ \vdots & \iddots & & \vdots \\ \mu_{n-1} & \cdots & \cdots & \mu_{2n-2} \end{bmatrix} \quad \text{and} \quad H_n^< := \begin{bmatrix} \mu_1 & \mu_2 & \cdots & \mu_n \\ \mu_2 & & \iddots & \vdots \\ \vdots & \iddots & & \vdots \\ \mu_n & \cdots & \cdots & \mu_{2n-1} \end{bmatrix}.$$

Theorem 2. *The eigenvalues of the pencil $H_n^< - \lambda H_n$ are given by $z_1, \ldots, z_n$.*

Therefore, we can obtain n distinct zeros of f by solving the generalized eigenvalue problem

$$H_n^< x = \lambda H_n x. \tag{3}$$

Note that the n mutually distinct zeros $z_1, \ldots, z_n$ are determined by the $2n$ moments $\mu_0, \mu_1, \ldots, \mu_{2n-1}$.

The value of n is determined indirectly. Once n and $z_1, \ldots, z_n$ have been found, the problem becomes linear and the multiplicities $v_1, \ldots, v_n$ can be computed by solving a Vandermonde system, cf. Eq. (1). As the multiplicities are known to be integers, this system does not need to be solved very accurately.

For further details about the algorithm, in particular concerning the use of formal orthogonal polynomials to improve the numerical stability, we refer to [9,10,12], in which also the case of clusters of zeros is considered and in which the connection with rational interpolation at roots of unity is explored. A Fortran 90 implementation of the algorithm is available (software package ZEAL) [15]. In [11] Kravanja and Van Barel presented a further generalization of this approach that does not require the derivative f'. In [13] they considered the related problem of computing all the zeros and poles (together with their respective multiplicities and orders) of a meromorphic function that lie inside a Jordan curve.

Torii and Sakurai [20] proposed a method to find zeros of an analytic function by using the extended Euclidean algorithm for polynomials constructed from the moments μ_p. Sakurai et al. [19]

applied this method in case f has dense clusters of zeros inside the unit circle. In these methods the Fast Fourier Transform was used to evaluate the moments.

Clustering methods for finding multiple or close zeros as clusters can be used to evaluate initial approximations and to improve convergence of factoring methods [2,17,18].

The integral that defines μ_p is an integral along a closed curve and hence, once the curve is parametrized and the integral is written as a Riemann integral, it is the integral of a periodic function along one period. The trapezoidal rule is therefore an appropriate quadrature rule [3,5,7,16]. Delves and Lyness as well as Kravanja et al. used this rule to calculate approximations for the moments.

In both quadrature methods that are obtained by (2) and (3) it was considered that the quadrature error directly affects the computed approximations of the zeros, and that hence it is necessary to evaluate the integrals sufficiently accurately. In this paper we present a detailed (forward and backward) error analysis in case the integrals are computed via the K-point trapezoidal rule on the unit circle. We show that, contrary to the Delves–Lyness method, the quadrature error that arises from the zeros located inside the unit circle does not affect the results of the approach of Kravanja et al. Numerical experiments illustrate our main conclusions.

2. Quadrature error of the moments

We will write $\mu_p(f)$ instead of simply μ_p whenever we want to emphasize the dependence on f. With obvious definitions of $\mu_p(P_N)$ and $\mu_p(g)$, the following holds:

$$\mu_p(f) = \mu_p(P_N) + \mu_p(g), \quad \mu_p(g) = 0.$$

In other words, only the contribution of P_N counts. Indeed, f and P_N have exactly the same zeros and corresponding multiplicities inside (and on) $\mathbb{T}$.

Let K be a positive integer. Then the Kth roots of unity are given by

$$\omega_j := e^{2\pi i/Kj}, \quad j = 0, 1, \ldots, K-1.$$

By approximating the integral that defines μ_p via the K-point trapezoidal rule (after having rewritten this integral as a Riemann integral over the interval $[0,1]$), one obtains the following approximation for μ_p:

$$\hat{\mu}_p = \hat{\mu}_p(f) := \frac{1}{K}\sum_{j=0}^{K-1} \omega_j^{p+1} \frac{f'(\omega_j)}{f(\omega_j)}.$$

Note that $\hat{\mu}_p = \hat{\mu}_{p+K}$ for all p and hence only $\hat{\mu}_0, \ldots, \hat{\mu}_{K-1}$ are relevant.

How good is this approximation? In the following paragraphs we will present a forward and backward error analysis.

Let us consider P_N'/P_N and g'/g in more detail. One can easily verify that the Laurent series at infinity of P_N'/P_N is given by

$$\frac{P_N'(z)}{P_N(z)} = \frac{\mu_0}{z} + \frac{\mu_1}{z^2} + \frac{\mu_2}{z^3} + \cdots .$$

The series converges for $|z| > \rho_I$, where

$$\rho_I := \max_{1 \leqslant k \leqslant n} |z_k| < 1.$$

(The subscript I stands for *interior*.) In other words, ρ_I is equal to the modulus of the zero(s) of f that lie(s) inside $\mathbb{T}$ and that is (are) closest to $\mathbb{T}$. As g'/g is analytic inside and on $\mathbb{T}$, it has a Taylor series expansion at the origin,

$$\frac{g'(z)}{g(z)} =: \gamma_0 + \gamma_1 z + \gamma_2 z^2 + \cdots .$$

The series converges for $|z| < \rho_E$ where $\rho_E > 1$ is defined as the modulus of the zero(s) or other singularities of f that lie(s) outside $\mathbb{T}$ and that is (are) closest to $\mathbb{T}$. (The subscript E stands for *exterior*.) By combining these two series expansions, we obtain the following important equation:

$$\frac{f'(z)}{f(z)} = \cdots + \frac{\mu_2}{z^3} + \frac{\mu_1}{z^2} + \frac{\mu_0}{z} + \gamma_0 + \gamma_1 z + \gamma_2 z^2 + \cdots .$$

for $\rho_I < |z| < \rho_E$. The series converges in a ring around the unit circle. In particular, it converges on $\mathbb{T}$ itself, for example for z equal to one of the Kth roots of unity.

With obvious definitions of $\hat{\mu}_p(P_N)$ and $\hat{\mu}_p(g)$, the following holds:

$$\hat{\mu}_p(f) = \hat{\mu}_p(P_N) + \hat{\mu}_p(g).$$

(Note that $\hat{\mu}_p(g)$ is an approximation of zero.) We consider the contributions of P_N and g separately.

Let us first consider $\hat{\mu}_p(P_N)$.

Theorem 3.

$$\hat{\mu}_p(P_N) = \sum_{r=0}^{+\infty} \mu_{p+rK}, \quad 0 \leqslant p \leqslant K-1.$$

Proof. The following holds:

$$\begin{aligned}
\hat{\mu}_p(P_N) &= \frac{1}{K} \sum_{j=0}^{K-1} \omega_j^{p+1} \frac{P_N'(\omega_j)}{P_N(\omega_j)} \\
&= \frac{1}{K} \sum_{j=0}^{K-1} \omega_j^{p+1} \left(\sum_{l=0}^{+\infty} \frac{\mu_l}{\omega_j^{l+1}} \right) \\
&= \sum_{l=0}^{+\infty} \mu_l \left(\frac{1}{K} \sum_{j=0}^{K-1} \omega_j^{p-l} \right) \\
&= \sum_{r=0}^{+\infty} \mu_{p+rK}
\end{aligned}$$

for $0 \leqslant p \leqslant K-1$. The last step follows from the fact that

$$\frac{1}{K}\sum_{j=0}^{K-1}\omega_j^{p-l} = \begin{cases} 1 & \text{if } p-l = rK \text{ for } r \in \mathbb{Z}, \\ 0 & \text{otherwise.} \end{cases} \tag{4}$$

This proves the theorem. □

The *forward approximation error* related to P_N is thus given by

$$\hat{\mu}_p(P_N) - \mu_p(P_N) = \hat{\mu}_p(P_N) - \mu_p = \mu_{p+K} + \mu_{p+2K} + \mu_{p+3K} + \cdots . \tag{5}$$

Note that the terms in the series on the right-hand side indeed converge to zero, which is a necessary condition for the series to converge. Also,

$$\hat{\mu}_p(P_N) - \mu_p = \mathcal{O}(\rho_I^{p+K}) \tag{6}$$

as follows from Eq. (1) and the definition of ρ_I. The approximation improves as K increases, as is to be expected, and the larger p or the smaller ρ_I, the better.

Let us now turn our attention to $\hat{\mu}_p(g)$.

Theorem 4.

$$\hat{\mu}_p(g) = \sum_{r=1}^{+\infty}\gamma_{rK-p-1}, \quad 0 \leqslant p \leqslant K-1.$$

Proof. The following holds:

$$\begin{aligned}\hat{\mu}_p(g) &= \frac{1}{K}\sum_{j=0}^{K-1}\omega_j^{p+1}\frac{g'(\omega_j)}{g(\omega_j)} \\ &= \frac{1}{K}\sum_{j=0}^{K-1}\omega_j^{p+1}\left(\sum_{l=0}^{+\infty}\gamma_l\omega_j^l\right) \\ &= \sum_{l=0}^{+\infty}\gamma_l\left(\frac{1}{K}\sum_{j=0}^{K-1}\omega_j^{p+l+1}\right) \\ &= \sum_{r=1}^{+\infty}\gamma_{rK-p-1}.\end{aligned}$$

The last step follows from relation (4). This proves the theorem. □

Note that $0 \leqslant p \leqslant K-1$ and that the summation starts with index $r=1$. This formula can be interpreted as follows. As g'/g is analytic inside and on $\mathbb{T}$, all its “negative” Laurent coefficients are equal to zero, in particular γ_{-p-1}, the coefficient belonging to the term $1/z^{p+1}$. This is the coefficient that the trapezoidal rule approximates. The approximation error is obtained by summing all the Laurent coefficients whose index is a (positive or negative) multiple of K away. The *forward approximation error* related to g is therefore given by

$$\hat{\mu}_p(g) - \mu_p(g) = \hat{\mu}_p(g) - 0 = \gamma_{K-p-1} + \gamma_{2K-p-1} + \gamma_{3K-p-1} + \cdots .$$

Since g'/g is analytic in the closed disk $\{z \in \mathbb{C} : |z| \leqslant \rho\}$, $1 < \rho < \rho_E$, it follows that

$$|\gamma_j| \leqslant \frac{M}{\rho^j}, \quad j = 0, 1, 2, \ldots,$$

where

$$M := \max_{|z|=\rho} \left| \frac{g'(z)}{g(z)} \right|.$$

It follows that

$$|\hat{\mu}_p(g)| \leqslant \sum_{r=1}^{+\infty} \frac{M}{\rho^{rK-p-1}} = M \frac{(\frac{1}{\rho})^{K-p-1}}{1-(\frac{1}{\rho})^K}.$$

Therefore,

$$\hat{\mu}_p(g) = \hat{\mu}_p(g) - \mu_p(g) = \mathcal{O}\left(\left(\frac{1}{\rho} \right)^{K-p-1} \right). \tag{7}$$

By combining Eqs. (6) and (7), we obtain our result concerning the forward approximation error.

Theorem 5. *For every $\rho \in \mathbb{R}$ such that $1 < \rho < \rho_E$, the following holds*:

$$\hat{\mu}_p(f) - \mu_p = \mathcal{O}(\rho_I^{p+K}) + \mathcal{O}(\rho^{p+1-K}).$$

Both P_N (via ρ_I) and g (via $\rho < \rho_E$) contribute to the approximation error. Note that, in a certain sense, these contributions work in opposite ways. More specifically, as far as the contribution of P_N is concerned, for fixed K, the *larger* p, the more accurate, while, as far as the contribution of g is concerned, again for fixed K, the *smaller* p, the more accurate. To obtain H_n and $H_n^<$ the moments $\mu_0, \mu_1, \ldots, \mu_{2n-1}$ are needed. Hence, the order of magnitude of μ_K and γ_{K-2n} determine the overall error.

3. Error analysis of the Kravanja–Sakurai–Van Barel method

In this section, we give an error analysis of the approach of Kravanja et al. The following theorem shows that, as far as the contribution of P_N is concerned, the fact that the moments are approximated via the trapezoidal rule has no effect at all, i.e., the generalized eigenvalues are still given by the zeros $z_1, \ldots, z_n$ (cf. Theorem 2). The corresponding multiplicities are obtained by solving a Vandermonde like linear system.

Define

$$\hat{H}_n(P_N) := [\hat{\mu}_{k+l}(P_N)]_{k,l=0}^{n-1} \quad \text{and} \quad \hat{H}_n^{<}(P_N) := [\hat{\mu}_{1+k+l}(P_N)]_{k,l=0}^{n-1}.$$

Theorem 6. *The eigenvalues of the pencil* $\hat{H}_n^{<}(P_N) - \lambda \hat{H}_n(P_N)$ *are given by* $z_1, \ldots, z_n$. *The corresponding multiplicities* $v_1, \ldots, v_n$ *are the solution of the linear system of equations*

$$\sum_{k=1}^{n} \left(\frac{z_k^p}{1 - z_k^K} \right) v_k = \hat{\mu}_p(P_N), \qquad p = 0, \ldots, n-1. \tag{8}$$

Proof. Let V_n be the Vandermonde matrix

$$V_n := \begin{bmatrix} 1 & \cdots & 1 \\ z_1 & \cdots & z_n \\ \vdots & & \vdots \\ z_1^{n-1} & \cdots & z_n^{n-1} \end{bmatrix}.$$

Note that V_n is nonsingular since $z_1, \ldots, z_n$ are mutually distinct.

From (1) and (5) it follows that

$$\begin{aligned} \hat{\mu}_p(P_N) &= \sum_{k=1}^{n} v_k z_k^p (1 + z_k^K + z_k^{2K} + \cdots) \\ &= \sum_{k=1}^{n} \left(\frac{v_k}{1 - z_k^K} \right) z_k^p, \end{aligned} \tag{9}$$

for $p = 0, 1, \ldots$. Let

$$\hat{v}_k := \frac{v_k}{1 - z_k^K}, \qquad k = 1, \ldots, n.$$

Define the diagonal matrices $\hat{D}_n$ and Z_n as

$$\hat{D}_n := \mathrm{diag}(\hat{v}_1, \ldots, \hat{v}_n) \quad \text{and} \quad Z_n := \mathrm{diag}(z_1, \ldots, z_n).$$

Then one can easily verify that

$$\hat{\mu}_p(P_N) = \sum_{k=1}^{n} \hat{v}_k z_k^p$$

implies that $\hat{H}_n(P_N)$ and $\hat{H}_n^{<}(P_N)$ can be factorized as follows:

$$\hat{H}_n(P_N) = V_n \hat{D}_n V_n^{\mathrm{T}} \quad \text{and} \quad \hat{H}_n^{<}(P_N) = V_n \hat{D}_n Z_n V_n^{\mathrm{T}}.$$

It follows that

$$\hat{H}_n^{<}(P_N) - \lambda \hat{H}_n(P_N) = V_n \hat{D}_n (Z_n - \lambda I_n) V_n^{\mathrm{T}}.$$

This proves the first part of the theorem. □

Eq. (9) immediately leads to the second part of the theorem.

Let us now investigate the influence of g in more detail. Define

$$\varphi_n(z) := \prod_{k=1}^{n}(z - z_k) =: z^n + u_{n-1}z^{n-1} + \cdots + u_1 z + u_0$$

and let $C_n \in \mathbb{C}^{n\times n}$ be the corresponding *companion matrix*

$$C_n := \begin{bmatrix} 0 & 0 & \cdots & 0 & -u_0 \\ 1 & 0 & \cdots & 0 & -u_1 \\ 0 & 1 & \ddots & \vdots & \vdots \\ \vdots & \ddots & \ddots & 0 & -u_{n-2} \\ 0 & 0 & \cdots & 1 & -u_{n-1} \end{bmatrix}.$$

From Theorems 2 and 6 one can easily verify that

$$H_n^< = H_n C_n \quad \text{and} \quad \hat{H}_n^<(P_N) = \hat{H}_n(P_N) C_n.$$

The computed approximations $\hat{z}_1, \ldots, \hat{z}_n$ of the zeros are given by the eigenvalues of the pencil $\hat{H}_n^<(f) - \lambda \hat{H}_n(f)$. Let

$$\hat{\varphi}_n(z) := \prod_{k=1}^{n}(z - \hat{z}_k)$$

and let $\hat{C}_n$ be the corresponding companion matrix. Then $\hat{H}_n^<(f) = \hat{H}_n(f)\hat{C}_n$.

Theorem 7. *If $\hat{H}_n(f)$ is nonsingular, then the following holds for every $\rho \in \mathbb{R}$ such that $1 < \rho < \rho_E$*

$$|\hat{\varphi}_n(z_k)| = \mathcal{O}(\rho^{2n-K}), \quad k = 1, \ldots, n.$$

Proof. Since $\hat{C}_n$ and C_n are the companion matrices of $\hat{\varphi}_n$ and φ_n, respectively,

$$\begin{pmatrix} \hat{\varphi}_n(z_1) \\ \vdots \\ \hat{\varphi}_n(z_n) \end{pmatrix} = -V_n^{\mathrm{T}} \hat{C}_n e_n + \begin{pmatrix} z_1^n \\ \vdots \\ z_n^n \end{pmatrix}$$

and

$$\begin{pmatrix} \varphi_n(z_1) \\ \vdots \\ \varphi_n(z_n) \end{pmatrix} = -V_n^{\mathrm{T}} C_n e_n + \begin{pmatrix} z_1^n \\ \vdots \\ z_n^n \end{pmatrix},$$

where $e_n := [0 \ \cdots \ 0 \ 1]^{\mathrm{T}}$. Hence

$$\begin{pmatrix} \hat{\varphi}_n(z_1) \\ \vdots \\ \hat{\varphi}_n(z_n) \end{pmatrix} - \begin{pmatrix} \varphi_n(z_1) \\ \vdots \\ \varphi_n(z_n) \end{pmatrix} = V_n^{\mathrm{T}}(C_n - \hat{C}_n)e_n$$

$$= V_n^{\mathrm{T}}\hat{H}_n^{-1}(\hat{H}_n C_n - \hat{H}_n^{<})e_n.$$

Since $\hat{H}_n^{<}(P_n) - \hat{H}_n(P_N)C_n = 0$ and $\varphi_n(z_k) = 0$, $k = 1, \ldots, n$, it follows that

$$\begin{pmatrix} \hat{\varphi}_n(z_1) \\ \vdots \\ \hat{\varphi}_n(z_n) \end{pmatrix} = V_n^{\mathrm{T}}\hat{H}_n^{-1}(\hat{H}_n(g)C_n - \hat{H}_n^{<}(g))e_n.$$

Therefore,

$$|\hat{\varphi}_n(z_k)| \leqslant \|V_n^{\mathrm{T}}\|_\infty \|\hat{H}_n^{-1}\|_\infty (\|\hat{H}_n(g)\|_\infty \|C_n e_n\|_\infty + \|\hat{H}_n^{<}(g)e_n\|_\infty)$$

for $k = 1, \ldots, n$. As $\hat{H}_n$ is nonsingular, the third factor on the right-hand side determines the order of magnitude. Let us investigate the norm of $\hat{H}_n(g)$. The following holds:

$$\begin{aligned} \|\hat{H}_n(g)\|_\infty &= \max_{0 \leqslant k \leqslant n-1} \sum_{l=0}^{n-1} |\hat{\mu}_{k+l}(g)| \\ &\leqslant \frac{M}{1-\rho^{-K}} \max_{0 \leqslant k \leqslant n-1} \sum_{l=0}^{n-1} \rho^{k+l+1-K} \\ &\leqslant \frac{M}{1-\rho^{-K}} \frac{\rho^n - 1}{\rho - 1} \rho^{n-K} \\ &= \mathcal{O}(\rho^{2n-K}). \end{aligned}$$

The last column of $\hat{H}_n^{<}(g)$ can be estimated in a similar way. It follows that

$$|\hat{\varphi}_n(z_k)| = \mathcal{O}(\rho^{2n-K}), \quad k = 1, \ldots, n.$$

This proves the theorem. □

Since the vector of the coefficients of $\hat{\varphi}_n - \varphi_n$ is given by $-\hat{C}_n e_n + C_n e_n$, it follows that

$$\|\hat{\varphi}_n - \varphi_n\| = \|(C_n - \hat{C}_n)e_n\|,$$

where the norm of a polynomial is defined as the (vector) norm of its vector of coefficients. The following result can be easily proved in as similar way as Theorem 7.

Theorem 8. *If $\hat{H}_n(f)$ is nonsingular, then the following holds for every $\rho \in \mathbb{R}$ such that $1 < \rho < \rho_E$*

$$\|\hat{\varphi}_n - \varphi_n\| = \mathcal{O}(\rho^{2n-K}).$$

Corollary 9. *$K \geqslant 2n$ is a necessary condition to obtain a small approximation error.*

In the case that some of zeros in $\mathbb{T}$ are very close, $\hat{H}_n(P_N)$ is close to singular. When the zeros of f in $\mathbb{T}$ can be grouped into m clusters, we can improve the condition of $\hat{H}_n(P_N)$ by considering a method to find m clusters instead of n zeros [10].

4. Numerical experiments

Let us now show the results of some numerical experiments. The algorithm was implemented in Matlab with double precision arithmetic.

Let $z_{1,K}^{\text{D–L}}, \ldots, z_{n,K}^{\text{D–L}}$ denote the approximate zeros obtained by the Delves–Lyness method where the moments are calculated via the K-point trapezoidal rule (at the Kth roots of unity). Similarly, let $z_{1,K}^{\text{K–S–V}}, \ldots, z_{n,K}^{\text{K–S–V}}$ denote the approximate zeros obtained by calculating the eigenvalues of the pencil $\hat{H}_n^{<}(f) - \lambda \hat{H}_n(f)$. (The superscript K–S–V refers to the authors of [10].) The multiplicities were calculated by solving the linear system of equations

$$\sum_{k=1}^{n} \left(\frac{(z_{k,K}^{\text{K–S–V}})^p}{1 - (z_{k,K}^{\text{K–S–V}})^K} \right) v_k = \hat{\mu}_p(f), \qquad p = 0, \ldots, n-1,$$

cf. Eq. (8) in Theorem 6.

Example 10. Suppose that

$$P_N(z) = (z - 0.2)^3 (z - 0.2 + 0.5i)(z - 0.2 - 0.5i)(z - 0.9)^2$$

and

$$g(z) = 1.$$

Observe that $\rho_I = 0.9$ and $\rho_E = \infty$. In Table 1 we show the results for various values of K.

In case $K = 8$, the computed approximations of the zeros $z_{1,8}^{\text{K–S–V}}, \ldots, z_{4,8}^{\text{K–S–V}}$ are given by

$$0.20000000000000 + 0.50000000000000i$$

$$0.20000000000000 - 0.50000000000000i$$

$$0.19999999999999 + 0.00000000000000i$$

$$0.90000000000000 + 0.00000000000000i$$

Table 1
Approximation errors for various values of K in Example 10

	$K=8$	$K=16$	$K=32$	$K=64$	$K=128$
$\max_{0\leqslant p\leqslant 2n-1} \lvert\hat{\mu}_p-\mu_p\rvert$	1.50e + 00	4.55e − 01	7.11e − 02	2.36e − 03	2.78e − 06
$\max_{1\leqslant j\leqslant n} \lvert z_{j,K}^{\text{D–L}}-z_j\rvert$	3.68e − 01	3.10e − 01	1.53e − 01	4.15e − 02	4.19e − 03
$\max_{1\leqslant j\leqslant n} \lvert z_{j,K}^{\text{K–S–V}}-z_j\rvert$	5.16e − 15	2.66e − 15	4.61e − 15	6.49e − 15	5.72e − 15

Table 2
Approximation errors for various values of K in Example 11

	$K=8$	$K=16$	$K=32$	$K=64$	$K=128$
$\max_{0\leqslant p\leqslant 2n-1} \lvert\hat{\mu}_p-\mu_p\rvert$	1.27e + 01	4.55e − 01	7.11e − 02	2.36e − 03	2.78e − 06
$\max_{1\leqslant j\leqslant n} \lvert z_{j,K}^{\text{D–L}}-z_j\rvert$	8.80e − 01	3.13e − 01	1.53e − 01	4.15e − 02	4.19e − 03
$\max_{1\leqslant j\leqslant n} \lvert z_{j,K}^{\text{K–S–V}}-z_j\rvert$	1.57e + 00	3.63e − 03	5.32e − 08	9.66e − 15	2.11e − 15

and the corresponding approximations of the multiplicities are given by

$$1.00000000000000 - 0.00000000000001i$$

$$1.00000000000000 + 0.00000000000001i$$

$$2.99999999999999 - 0.00000000000000i$$

$$2.00000000000001 + 0.00000000000000i.$$

Since $g=1$, only P_N plays a role and the computed approximations are very accurate, cf. Theorem 6.

Example 11. Suppose that

$$P_N(z) = (z-0.2)^3(z-0.2+0.5i)(z-0.2-0.5i)(z-0.9)^2$$

and

$$g(z) = (z-2)(z-3)(z-4)(z-5)\exp(5z^3+2z^4+z^5).$$

Observe that $\rho_I = 0.9$ and $\rho_E = 2$. In Table 2 we show the results for various values of K. In case $K=16$, the computed approximations of the zeros are given by

$$0.20116264354169 + 0.50032172670692i$$

$$0.20116264354169 - 0.50032172670692i$$

$$0.19637048394944 + 0.00000000000000i$$

$$0.89943464186948 + 0.00000000000000i$$

and the corresponding computed approximations of the multiplicities are given by

$$0.99381191467514 - 0.00479762188495i$$

$$0.99381191467514 + 0.00479762188495i$$

$$3.00545283047740 - 0.00000000000000i$$

$$2.01018978549059 + 0.00000000000000i.$$

In case $K = 64$, the computed approximations of the zeros are given by

$$0.20000000000000 + 0.50000000000000i$$

$$0.20000000000000 - 0.50000000000000i$$

$$0.19999999999999 + 0.00000000000000i$$

$$0.89999999999999 + 0.00000000000000i$$

and the corresponding computed approximations of the multiplicities are given by

$$0.99999999999999 - 0.00000000000001i$$

$$0.99999999999999 + 0.00000000000001i$$

$$2.99999999999998 - 0.00000000000000i$$

$$1.99999999999992 + 0.00000000000000i.$$

Acknowledgements

This research was partially supported by the K.U. Leuven (Bijzonder Onderzoeksfonds), project "SLAP: Structured Linear Algebra Package," Grant OT/00/16.

References

[1] M.P. Carpentier, A.F. Dos Santos, Solution of equations involving analytic functions, J. Comput. Phys. 45 (1982) 210–220.
[2] C. Carstensen, T. Sakurai, Simultaneous factorization of a polynomial by rational approximation, J. Comput. Appl. Math. 61 (2) (1995) 165–178.
[3] P.J. Davis, P. Rabinowitz, Methods of Numerical Integration, Academic Press, New York, 1984.
[4] L.M. Delves, J.N. Lyness, A numerical method for locating the zeros of an analytic function, Math. Comput. 21 (1967) 543–560.
[5] R.J. Fornaro, Numerical evaluation of integrals around simple closed curves, SIAM J. Numer. Anal. 10 (4) (1973) 623–634.
[6] P. Henrici, Applied and Computational Complex Analysis: I. Power Series—Integration—Conformal Mapping—Location of Zeros, Wiley, New York, 1974.
[7] D.B. Hunter, The evaluation of integrals of periodic analytic functions, BIT 11 (1971) 175–180.
[8] N.I. Ioakimidis, Quadrature methods for the determination of zeros of transcendental functions—a review, in: P. Keast, G. Fairweather (Eds.), Numerical Integration: Recent Developments, Software and Applications, Reidel, Dordrecht, The Netherlands, 1987, pp. 61–82.
[9] P. Kravanja, On computing zeros of analytic functions and related problems in structured numerical linear algebra, Ph.D. Thesis, Katholieke Universiteit Leuven, Department of Computer Science, 1999.

[10] P. Kravanja, T. Sakurai, M. Van Barel, On locating clusters of zeros of analytic functions, BIT 39 (4) (1999) 646–682.
[11] P. Kravanja, M. Van Barel, A derivative-free algorithm for computing zeros of analytic functions, Computing 63 (1) (1999) 69–91.
[12] P. Kravanja, M. Van Barel, Computing the zeros of analytic functions, Lecture Notes in Mathematics, Vol. 1727, Springer, Berlin, 2000.
[13] P. Kravanja, M. Van Barel, A. Haegemans, On computing zeros and poles of meromorphic functions, in: N. Papamichael, St. Ruscheweyh, E.B. Saff (Eds.), Computational Methods and Function Theory Series in Approximations and Decompositions, Vol. 11, World Scientific, Singapore, 1999, Proceedings of the third CMFT Conference, Nicosia, 1997, pp. 359–369.
[14] P. Kravanja, M. Van Barel, A. Haegemans, Logarithmic residue based methods for computing zeros of analytic functions and related problems, in: E.A. Lipitakis (Ed.), HERCMA '98: Proceedings of the Fourth Hellenic-European Conference on Computer Mathematics and its Applications, Athens, LEA, 1999, pp. 201–208.
[15] P. Kravanja, M. Van Barel, O. Ragos, M.N. Vrahatis, F.A. Zafiropoulos, ZEAL: a mathematical software package for computing zeros of analytic functions, Comput. Phys. Commun. 124 (2–3) (2000) 212–232.
[16] J.N. Lyness, L.M. Delves, On numerical contour integration round a closed contour, Math. Comput. 21 (1967) 561–577.
[17] T. Sakurai, H. Sugiura, On factorization of analytic functions and its verification, Reliable Comput. 6 (4) (2000) 459–470.
[18] T. Sakurai, H. Sugiura, Improvement of convergence of an iterative method for finding polynomial factors of analytic functions, J. Comput. Appl. Math. 140 (1–2) (2002) 713–726.
[19] T. Sakurai, T. Torii, N. Ohsako, H. Sugiura, A method for finding clusters of zeros of analytic function, Special Issues of Zeitschrift für Angewandte Mathematik und Mechanik (ZAMM). Issue 1: Numerical Analysis, Scientific Computing, Computer Science, 1996, Proceedings of the International Congress on Industrial and Applied Mathematics (ICIAM/GAMM 95), Hamburg, 1995, pp. 515–516.
[20] T. Torii, T. Sakurai, Global method for the poles of analytic function by rational interpolant on the unit circle, World Sci. Ser. Appl. Anal. 2 (1993) 389–398.
[21] X. Ying, I.N. Katz, A reliable argument principle algorithm to find the number of zeros of an analytic function in a bounded domain, Numer. Math. 53 (1988) 143–163.