Logarithmic residue based methods for computing zeros of analytic functions and related problems

P. Kravanja*, M. Van Barel and A. Haegemans
Department of Computer Science, Katholieke Universiteit Leuven
Celestijnenlaan 200 A, B-3001 Heverlee (Belgium)

Abstract

Given an analytic function f and a positively oriented Jordan curve γ, we consider the problem of computing all the zeros of f that lie inside γ, together with their respective multiplicities. By exploiting the connection between logarithmic residue integrals and the theory of formal orthogonal polynomials, we obtain an accurate algorithm that proceeds by solving generalized eigenvalue problems and a Vandermonde system. We show how similar techniques can be applied to the following problems: computing zeros and poles of meromorphic functions and locating clusters of zeros of analytic functions.

1 Introduction

Let W be a simply connected region in $\mathbb{C}$, $f : W \to \mathbb{C}$ analytic in W, and γ a positively oriented Jordan curve in W that does not pass through any zero of f. We consider the problem of computing *all* the zeros of f that lie in the interior of γ, together with their respective multiplicities.

Let N denote the total number of zeros of f that lie in the interior of γ, i.e., the number of zeros where each zero is counted according to its multiplicity. Suppose that $N > 0$. Let the sequence $Z_1, \ldots, Z_N$ consist of all the zeros of f that lie inside γ. Each zero is repeated according to its multiplicity. 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. It follows that

$$N = \frac{1}{2\pi i} \int_\gamma \frac{f'(z)}{f(z)}\, dz$$

and thus N can be calculated via numerical integration. Integrals of this type are called *logarithmic residue integrals*. 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 is given in [8]. A classical approach is to consider the integrals

$$s_p := \frac{1}{2\pi i} \int_\gamma z^p \frac{f'(z)}{f(z)}\, dz, \qquad p = 0, 1, 2, \ldots.$$

*Corresponding author. E-mail: Peter.Kravanja@na-net.ornl.gov

$$s_p = Z_1^p + \cdots + Z_N^p, \qquad p = 0, 1, 2, \ldots. \tag{1}$$

Delves and Lyness [4] considered the monic polynomial $P_N(z)$ of degree N that has zeros $Z_1, \ldots, Z_N$ and calculated its coefficients via Newton's identities. In this way they reduced the problem to the easier problem of computing the zeros of a polynomial. Unfortunately, the map from the Newton sums to the coefficients (in the standard monomial basis) of $P_N(z)$ 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. The location of the zeros determines their sensitivity to perturbations of the coefficients. Multiple zeros and very close zeros are extremely sensitive, but even a succession of moderately close zeros can result in severe ill-conditioning. The composite map (from the Newton sums to the zeros and their respective multiplicities) is also usually ill-conditioned.

A similar approach was taken by Li [11] who considered (1) as a system of polynomial equations. Li used a homotopy continuation method to solve this system.

What is wrong with these approaches, in our opinion, is that they consider the wrong set of unknowns. One should consider the mutually distinct zeros and their respective multiplicities separately. Let n denote the number of mutually distinct zeros of f that lie in the interior of γ. Let $z_1, \ldots, z_n$ be these zeros and $\nu_1, \ldots, \nu_n$ their respective multiplicities. In Section 2 we will show how these unknowns can be calculated by solving generalized eigenvalue problems and a Vandermonde system. Our approach exploits the connection between logarithmic residue integrals and the theory of formal orthogonal polynomials. In Section 3 we show how similar techniques can be applied to the following problems: computing zeros and poles of meromorphic functions and locating clusters of zeros of analytic functions.

2 Formal orthogonal polynomials

Let $\mathcal{P}$ be the linear space of polynomials with complex coefficients. We define a symmetric bilinear form $\langle \cdot, \cdot \rangle : \mathcal{P} \times \mathcal{P} \to \mathbb{C}$ by setting

$$\langle \phi, \psi \rangle := \frac{1}{2\pi i} \int_\gamma \phi(z)\psi(z)\frac{f'(z)}{f(z)}\, dz = \sum_{k=1}^{n} \nu_k \phi(z_k)\psi(z_k)$$

for any two polynomials $\phi, \psi \in \mathcal{P}$. Note that $\langle \cdot, \cdot \rangle$ can be evaluated via numerical integration.

A monic polynomial φ_t of degree $t \geq 0$ that satisfies

$$\langle z^k, \varphi_t(z) \rangle = 0, \qquad k = 0, 1, \ldots, t-1, \tag{2}$$

is called a *formal orthogonal polynomial* (FOP) of degree t. (Observe that condition (2) is void for $t = 0$.) The adjective *formal* emphasizes the fact that, in general, the form $\langle \cdot, \cdot \rangle$ does not define a true inner product. An important consequence of this fact is that, in contrast to polynomials that are orthogonal with respect to a true inner product, FOPs φ_t need not exist or need not be unique for every degree t. (For details, see for example [7] and the references cited therein.) If (2) is satisfied and φ_t is unique, then φ_t is called a *regular* FOP and t a *regular index*. If we set

$$\varphi_t(z) =: u_{0,t} + u_{1,t} z + \cdots + u_{t-1,t} z^{t-1} + z^t$$

$$\begin{bmatrix} s_0 & s_1 & \cdots & s_{t-1} \\ s_1 & & \iddots & \vdots \\ \vdots & \iddots & & \vdots \\ s_{t-1} & \cdots & \cdots & s_{2t-2} \end{bmatrix} \begin{bmatrix} u_{0,t} \\ u_{1,t} \\ \vdots \\ u_{t-1,t} \end{bmatrix} = - \begin{bmatrix} s_t \\ s_{t+1} \\ \vdots \\ s_{2t-1} \end{bmatrix}. \tag{3}$$

Hence, the regular FOP of degree $t \geq 1$ exists if and only if the Hankel matrix $H_t := [s_{k+l}]_{k,l=0}^{t-1}$ is regular. Thus, the rank profile of $H := [s_{k+l}]_{k,l\geq 0}$ determines which regular FOPs exist.

Theorem 1 *$n = \operatorname{rank} H_{n+p}$ for every integer $p \geq 0$. In particular, $n = \operatorname{rank} H_N$.*

Proof. Let p be a nonnegative integer. As

$$s_p = \langle 1, z^p \rangle = \sum_{k=1}^{n} \nu_k z_k^p$$

for $p = 0, 1, 2, \ldots$, the matrix H_{n+p} can be written as

$$H_{n+p} = \sum_{k=1}^{n} \nu_k \mathbf{z}_k \mathbf{z}_k^T \qquad \text{where } \mathbf{z}_k := \begin{bmatrix} 1 & z_k & \cdots & z_k^{n+p-1} \end{bmatrix}^T.$$

This implies that $\operatorname{rank} H_{n+p} \leq n$. However, H_n is regular. Indeed, one can easily verify that H_n can be factorized as $H_n = V_n D_n V_n^T$ where V_n is the Vandermonde matrix $V_n := [\, z_s^{r-1} \,]_{r,s=1}^{n}$ and D_n is the diagonal matrix $D_n := \operatorname{diag}(\nu_1, \ldots, \nu_n)$. Therefore $\operatorname{rank} H_{n+p} \geq n$. It follows that $\operatorname{rank} H_{n+p} = n$. □

By assumption $s_0 = N \neq 0$, and thus the regular FOP of degree 1 exists. It is given by $\varphi_1(z) = z - \mu$ where $\mu := s_1/s_0$. Theorem 1 implies that the regular FOP φ_n of degree n exists and tells us also that regular FOPs of degree larger than n do not exist. The polynomial φ_n is easily seen to be

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

It is the monic polynomial of degree n that has $z_1, \ldots, z_n$ as simple zeros.

If H_n is strongly regular, i.e., if all its leading principal submatrices are regular, then we have a full set $\{\varphi_0, \varphi_1, \ldots, \varphi_n\}$ of regular FOPs.

What happens if H_n is not strongly regular? By filling up the gaps in the sequence of existing regular FOPs it is possible to define a sequence $\{\varphi_t\}_{t=0}^{\infty}$, with φ_t a monic polynomial of degree t, such that if these polynomials are grouped into blocks according to the sequence of regular indices, then polynomials belonging to different blocks are orthogonal with respect to $\langle \cdot, \cdot \rangle$. More precisely, define $\{\varphi_t\}_{t=0}^{\infty}$ as follows. If t is a regular index, then let φ_t be the regular FOP of degree t. Else define φ_t as $\varphi_r \psi_{t,r}$ where r is the largest regular index less than t and $\psi_{t,r}$ is an arbitrary monic polynomial of degree $t - r$. In the latter case φ_t is called an *inner polynomial*. If $\psi_{t,r}(z) = z^{t-r}$ then we say that φ_t is defined *by using the standard monomial basis*. These polynomials $\{\varphi_t\}_{t=0}^{\infty}$ can be grouped into blocks. Each block starts with a regular FOP and the remaining polynomials are inner polynomials. Note that the last block has infinite length.

The so-called *block orthogonality* property is expressed by the fact that the Gram matrix $G_n := [\langle \varphi_r, \varphi_s \rangle]_{r,s=0}^{n-1}$ is block diagonal. The diagonal blocks are regular, symmetric and zero above the main antidiagonal. If all the inner polynomials in a certain block are defined by using the standard

$[\langle\varphi_r, \varphi_1\varphi_s\rangle]_{r,s=0}^{n-1}$ is block tridiagonal. The diagonal blocks are symmetric and lower anti-Hessenberg (i.e., its entries are equal to zero along all the antidiagonals that lie above the main antidiagonal, except for the antidiagonal that precedes the main antidiagonal). Again, if all the inner polynomials in a certain block are defined by using the standard monomial basis, then the corresponding diagonal block is a Hankel matrix. The entries of the off-diagonal blocks are all equal to zero, except for the entry in the south-east corner. For proofs and further details, we refer to [2].

Theorem 2 *The eigenvalues of the pencil $G_n^{(1)} - \lambda G_n$ are $\varphi_1(z_1), \ldots, \varphi_1(z_n)$. In other words, they are given by $z_1 - \mu, \ldots, z_n - \mu$ where $\mu = s_1/s_0$.*

Proof. Define V_n as the Vandermonde-like matrix $V_n := [\varphi_r(z_s)]_{r=0,s=1}^{n-1,n}$ and let D_n and $D_n^{(1)}$ be the diagonal matrices $D_n := \mathrm{diag}(\nu_1, \ldots, \nu_n)$ and $D_n^{(1)} := \mathrm{diag}(\nu_1\varphi_1(z_1), \ldots, \nu_n\varphi_1(z_n))$. Then G_n and $G_n^{(1)}$ can be factorized as $G_n = V_n D_n V_n^T$ and $G_n^{(1)} = V_n D_n^{(1)} V_n^T$. Let $\lambda^\star$ be an eigenvalue of the pencil $G_n^{(1)} - \lambda G_n$ and x a corresponding eigenvector. Then

$$\begin{aligned}
& G_n^{(1)}x = \lambda^\star G_n x \\
\Leftrightarrow \quad & (V_n D_n^{(1)} V_n^T)x = \lambda^\star (V_n D_n V_n^T)x \\
\Leftrightarrow \quad & D_n^{(1)} y = \lambda^\star D_n y \quad \text{if } y := V_n^T x \\
\Leftrightarrow \quad & \mathrm{diag}(\varphi_1(z_1), \ldots, \varphi_1(z_n))y = \lambda^\star y.
\end{aligned}$$

This proves the theorem. □

If n and $\varphi_0, \varphi_1, \ldots, \varphi_{n-1}$ are known, then we can apply the previous theorem to obtain $z_1, \ldots, z_n$. By Theorem 1 the value of n can be computed as the rank of H_N, but this is not a very practical approach. Instead, we will start to compute the polynomials $\{\varphi_t\}_{t=0}^{\infty}$ one by one and determine the value of n as the degree of the last existing regular FOP. The upper bound N will play a crucial role in the computations.

Theorem 2 can be interpreted as follows: the zeros of the nth degree regular FOP can be calculated by solving a generalized eigenvalue problem. This property holds for *all* regular FOPs. This will enable us to compute regular FOPs in their product representation, which is numerically very stable. Define the matrices G_k and $G_k^{(1)}$ as

$$G_k := [\langle\varphi_r, \varphi_s\rangle]_{r,s=0}^{k-1} \qquad \text{and} \qquad G_k^{(1)} := [\langle\varphi_r, \varphi_1\varphi_s\rangle]_{r,s=0}^{k-1}$$

for $k = 1, 2, \ldots$.

Theorem 3 *Let $t \geq 1$ be a regular index and let $z_{t,1}, \ldots, z_{t,t}$ be the zeros of the regular FOP φ_t. Then the eigenvalues of the pencil $G_t^{(1)} - \lambda G_t$ are given by $\varphi_1(z_{t,1}), \ldots, \varphi_1(z_{t,t})$. In other words, they are given by $z_{t,1} - \mu, \ldots, z_{t,t} - \mu$ where $\mu = s_1/s_0$.*

Proof. Define the Hankel matrix $H_t^<$ as $H_t^< := [s_{1+k+l}]_{k,l=0}^{t-1}$. We will first show that the zeros of φ_t are given by the eigenvalues of the pencil $H_t^< - \lambda H_t$. The zeros of φ_t are given by the eigenvalues of its companion matrix C_t. Let $\lambda^\star$ be an eigenvalue of C_t and x a corresponding eigenvector. As H_t is regular, we may conclude that $C_t x = \lambda^\star x \Leftrightarrow H_t C_t x = \lambda^\star H_t x$. Using (3) one can easily verify that $H_t C_t = H_t^<$.

Then G_t can be factorized as $G_t = A_t^T H_t A_t$. As $\varphi_1(z) = z - \mu$ where $\mu = s_1/s_0$, the matrix $G_t^{(1)}$ is given by $[\langle \varphi_r, z\varphi_s \rangle]_{r,s=0}^{t-1} - \mu G_t$. The matrix $[\langle \varphi_r, z\varphi_s \rangle]_{r,s=0}^{t-1}$ can be written as $A_t^T H_t^< A_t$ and thus $G_t^{(1)} = A_t^T (H_t^< - \mu H_t) A_t$. Now let $\lambda^\star$ be an eigenvalue of the pencil $H_t^< - \lambda H_t$ and x a corresponding eigenvector. Then

$$
\begin{aligned}
& H_t^< x = \lambda^\star H_t x \\
\Leftrightarrow \quad & (H_t^< - \mu H_t) x = (\lambda^\star - \mu) H_t x \\
\Leftrightarrow \quad & A_t^T (H_t^< - \mu H_t) A_t y = \varphi_1(\lambda^\star) A_t^T H_t A_t y \quad \text{if } y := A_t^{-1} x \\
\Leftrightarrow \quad & G_t^{(1)} y = \varphi_1(\lambda^\star) G_t y.
\end{aligned}
$$

This proves the theorem. □

Regular FOPs are characterized by the fact that the determinant of a Hankel matrix is different from zero, while inner polynomials correspond to singular Hankel matrices. By using an explicit determinant expression for regular FOPs, one can show that $\langle \varphi_t, \varphi_t \rangle = \det H_{t+1} / \det H_t$. Therefore, if t is a regular index, then $t+1$ is a regular index if and only if $\langle \varphi_t, \varphi_t \rangle \neq 0$. However, from a numerical point of view a test "is equal to zero" does not make sense. Because of rounding errors in the evaluation of $\langle \cdot, \cdot \rangle$ we would encounter only regular FOPs. Strictly speaking one could say that inner polynomials are not needed in numerical calculations. However, the opposite is true! Let us call a regular FOP *well-conditioned* if its corresponding Yule-Walker system (3) is well-conditioned, and *ill-conditioned* otherwise. To obtain a numerically stable algorithm, it is crucial to generate only well-conditioned regular FOPs and to replace ill-conditioned regular FOPs by inner polynomials. Stable look-ahead solvers for linear systems of equations that have Hankel structure are based on this principle [1, 3, 5]. In this approach the diagonal blocks in G_n are taken (slightly) larger than strictly necessary to avoid ill-conditioned blocks. A disadvantage is that part of the structure of G_n and $G_n^{(1)}$ gets lost and that there will be some additional fill-in.

We will ask the user for two thresholds, ϵ_{stop} and ϵ_{cond} with $\epsilon_{\text{stop}} < \epsilon_{\text{cond}}$, to decide whether the algorithm may stop or not, and to determine the size of a block. Suppose that the algorithm has just generated a well-conditioned regular FOP φ_r. If $r = N$, then we may stop. Else we proceed to calculate $\langle \varphi_r, \varphi_r \rangle$. If $|\langle \varphi_r, \varphi_r \rangle| \geq \epsilon_{\text{cond}}$ then we generate φ_{r+1} as a regular FOP, i.e., we solve a generalized eigenvalue problem to obtain the zeros of φ_{r+1}. Else we scan the sequence $(|\langle z^t \varphi_r, \varphi_r \rangle|)_{t=0}^{N-1-r}$. If $|\langle z^t \varphi_r, \varphi_r \rangle| < \epsilon_{\text{stop}}$ for $t = 0, 1, \ldots, N-1-r$ then we conclude that $n = r$ and stop. Else we search for the first element that is larger than ϵ_{cond}. The corresponding value of t then determines the size of the block of polynomials. If all the elements are less than ϵ_{cond} then we use the value of t that corresponds to the maximum to determine the block size and warn the user that we could not obtain the level of well-conditioning that he or she requested.

Once approximations for the zeros have been calculated, the multiplicities can be found by solving the Vandermonde system

$$
\begin{bmatrix} 1 & \cdots & 1 \\ z_1 & \cdots & z_n \\ \vdots & & \vdots \\ z_1^{n-1} & \cdots & z_n^{n-1} \end{bmatrix} \begin{bmatrix} \nu_1 \\ \nu_2 \\ \vdots \\ \nu_n \end{bmatrix} = \begin{bmatrix} s_0 \\ s_1 \\ \vdots \\ s_{n-1} \end{bmatrix}.
$$

accurate results. Note that it does not require initial guesses for the zeros. Also, as not only approximations for the zeros are computed but also the corresponding multiplicities, one can use the quadratically convergent modified Newton's iteration to refine the approximations for the zeros.

3 Related problems

3.1 Computing zeros and poles of meromorphic functions

Let W and γ be defined as above, and let $f : W \to \mathbb{C}$ be meromorphic in W. Suppose that f has neither zeros nor poles on γ. We consider the problem of computing *all* the zeros and poles of f that lie in the interior of γ, together with their respective multiplicities and orders. Let N denote the total number of zeros of f that lie inside γ, and let P denote the total number of poles of f that lie inside γ. Suppose that $N + P > 0$. Let n denote the number of mutually distinct zeros of f that lie inside γ. Let $z_1, \ldots, z_n$ be these zeros and $\nu_1, \ldots, \nu_n$ their respective multiplicities. Let p denote the number of mutually distinct poles of f that lie inside γ. Let $y_1, \ldots, y_p$ be these poles and $\mu_1, \ldots, \mu_p$ their respective orders. The logarithmic derivative $f'(z)/f(z)$ has a simple pole at z_k with residue ν_k for $k = 1, \ldots, n$ and a simple pole at y_l with residue $-\mu_l$ for $l = 1, \ldots, p$. It follows that

$$\langle \phi, \psi \rangle := \frac{1}{2\pi i} \int_\gamma \phi(z)\psi(z)\frac{f'(z)}{f(z)}\,dz = \sum_{k=1}^{n} \nu_k \phi(z_k)\psi(z_k) - \sum_{l=1}^{p} \mu_l \phi(y_l)\psi(y_l)$$

for any two polynomials $\phi, \psi \in \mathcal{P}$. The FOP of degree $n + p$ with respect to this form is given by

$$\prod_{k=1}^{n}(z - z_k)\prod_{l=1}^{p}(z - y_l). \tag{4}$$

Our algorithm for computing zeros of analytic functions is essentially an algorithm for computing zeros of FOPs. Provided that an upper bound for $n + p$ is known, one can easily verify that the algorithm can be modified to compute the zeros of (4), i.e., the mutually distinct zeros and poles of f that lie inside γ. Once these have been calculated, their corresponding multiplicities and orders can be calculated by solving a Vandermonde system. The sign of a component of the solution of this systems tells us whether the corresponding zero of the FOP of degree $n + p$ is a zero of f or a pole.

As $s_0 := \langle 1, 1 \rangle = N - P$ can be computed via numerical integration and $n + p \leq N + P = s_0 + 2P$ it follows that an upper bound for P immediately leads to the required upper bound for $n + p$. In case γ is the unit circle, such a bound for P can be obtained by using the heuristic approach of Gleyse and Kaliaguine [6].

3.2 Locating clusters of zeros of analytic functions

Suppose that f is analytic and suppose that the zeros of f that lie inside γ can be grouped into m clusters. In this case, the problem of computing all the zeros of f that lie inside γ is notoriously ill-conditioned. Let $I_1, \ldots, I_m$ be index sets that define these clusters, and let

$$\mu_j := \sum_{k \in I_j} \nu_k \quad \text{and} \quad c_j := \frac{1}{\mu_j} \sum_{k \in I_j} \nu_k z_k$$

(its "weight") whereas c_j is equal to the arithmetic mean of the zeros in cluster j (its "centre of gravity"). We will show how our algorithm for computing zeros of analytic functions can be used to obtain approximations for the centres $c_1, \ldots, c_m$ of the clusters, together with the corresponding weights $\mu_1, \ldots, \mu_m$. This information enables one to zoom into a certain cluster: its zeros can be calculated separately from the other zeros of f. By shifting the origin in the complex plane to the centre of a certain cluster, its zeros become better relatively separated, which is appropriate in floating point arithmetic and reduces the ill-conditioning.

For $k = 1, \ldots, n$ we define $\zeta_k := z_k - c_j$ if $k \in I_j$. From the definition of μ_j and c_j it follows that

$$\sum_{k \in I_j} \nu_k \zeta_k = 0, \qquad j = 1, \ldots, m. \tag{5}$$

Define the symmetric bilinear form $\langle \cdot, \cdot \rangle_m$ by

$$\langle \phi, \psi \rangle_m := \sum_{j=1}^{m} \mu_j \phi(c_j) \psi(c_j)$$

for any two polynomials $\phi, \psi \in \mathcal{P}$. This form is related to the form $\langle \cdot, \cdot \rangle$ in an obvious way: instead of the zeros $z_1, \ldots, z_n$ and their multiplicities $\nu_1, \ldots, \nu_n$ we now use the centres of gravity $c_1, \ldots, c_m$ and the weights $\mu_1, \ldots, \mu_m$ of the clusters. Let

$$\delta := \max_{1 \le k \le n} |\zeta_k|.$$

The following theorem tells us that $\langle \cdot, \cdot \rangle_m$ approximates $\langle \cdot, \cdot \rangle$ (and vice versa).

Theorem 4 *Let $\phi, \psi \in \mathcal{P}$. Then $\langle \phi, \psi \rangle = \langle \phi, \psi \rangle_m + \mathcal{O}(\delta^2), \delta \to 0$.*

Proof. This follows immediately by expanding the terms in

$$\langle \phi, \psi \rangle = \sum_{k=1}^{n} \nu_k \phi(z_k) \psi(z_k) = \sum_{j=1}^{m} \sum_{k \in I_j} \nu_k \phi(c_j + \zeta_k) \psi(c_j + \zeta_k)$$

into a Taylor series and by taking into account equation (5). □

In other words, if δ is sufficiently small, then we can expect our algorithm for computing zeros of analytic functions to behave as if the underlying symmetric bilinear form is $\langle \cdot, \cdot \rangle_m$ instead of $\langle \cdot, \cdot \rangle$. The FOP of degree m will be a regular FOP and its zeros will be good approximations for the centres $c_1, \ldots, c_m$. The FOPs of degree larger than m will be ill-conditioned. The following result confirms this intuition.

Corollary 5 *The matrix H_m is regular if $\delta \to 0$. Let $t > m$. Then $\det H_t = \mathcal{O}(\delta^2)$, $\delta \to 0$.*

Let $\varphi_m(z)$ be the FOP of degree m with respect to the form $\langle \cdot, \cdot \rangle$. Then $\varphi_m(c_j) = \mathcal{O}(\delta^2)$, $\delta \to 0$ for $j = 1, \ldots, m$. Also $\langle z^p, \varphi_m(z) \rangle = \mathcal{O}(\delta^2)$, $\delta \to 0$ for all $p \ge m$.

Once approximations for the centres have been found, the corresponding weights can be calculated by solving a Vandermonde system. For more details, including a proof of the previous corollary, numerical examples as well as a different approach based on rational interpolation at roots of unity, we refer to [10].

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