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A perturbation result for generalized eigenvalue problems and its application to error estimation in a quadrature method for computing zeros of analytic functions

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Abstract

We consider the quadrature method developed by Kravanja et al. (BIT 39 (4) (1999) 646) for computing all the zeros of an analytic function that lie inside the unit circle. A new perturbation result for generalized eigenvalue problems allows us to obtain a detailed upper bound for the error between the zeros and their approximations. To the best of our knowledge, it is the first time that such an error estimate is presented for any quadrature method for computing zeros of analytic functions. Numerical experiments illustrate our results.

MSC: 65H05

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

1. Introduction

For some years now, the authors have been working on the problem of computing *all* the zeros of an analytic function that lie inside a Jordan curve (say, the unit circle), together with their respective multiplicities [2,3].

Our paper [5] contains some of our most recent contributions to this research subject. However, this publication was allowed only a limited number of pages. We would now like to add some

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more results. The current paper should thus be read as a follow-up to [5]. We have chosen to avoid (lengthy) repetition of notations, preliminary results and bibliographical references. Whereas [5] contains only theorems stating that the analytic function evaluated at the approximate zeros is of a given small order of magnitude, we will now present a detailed upper bound for the error between the zeros and their approximations as computed by the algorithm of Kravanja, Sakurai & Van Barel. To the best of our knowledge, it is the first time that such an error estimate is presented for any quadrature method for computing zeros of analytic functions.

2. Sensitivity of generalized eigenvalue problems

This error estimate will be derived from a perturbation result for generalized eigenvalue problems. Although similar results exist, we have not come across this particular one in the literature. As we hope that it might be of interest beyond the particular setting of computing zeros of analytic functions, we formulate our perturbation result in general terms.

Let us consider the pencil $A - \lambda B$ where A and B are square complex matrices. The matrix B is assumed to be nonsingular and the eigenvalue, which we also denote by λ, is assumed to be simple.

Let the vectors x and v be the corresponding right and left eigenvectors,

$$Ax = \lambda Bx \quad \text{and} \quad v^{\mathrm{T}}A = \lambda v^{\mathrm{T}}B.$$

We consider the following perturbed problem:

$$(A + \varepsilon F)x(\varepsilon) = \lambda(\varepsilon)(B + \varepsilon G)x(\varepsilon)$$

where $\|F\| = \|G\| = 1$. As B is nonsingular and λ is a simple eigenvalue, standard results from function theory (see, e.g., [1, p. 63]) imply that $x(\varepsilon)$ and $\lambda(\varepsilon)$ are differentiable in a neighbourhood of $\varepsilon = 0$.

By differentiating with respect to ε we obtain:

$$\begin{aligned} &A\dot{x}(\varepsilon) + Fx(\varepsilon) + \varepsilon F\dot{x}(\varepsilon) \\ &\quad = \lambda(\varepsilon)B\dot{x}(\varepsilon) + \dot{\lambda}(\varepsilon)Bx(\varepsilon) + \lambda(\varepsilon)\varepsilon G\dot{x}(\varepsilon) + \lambda(\varepsilon)Gx(\varepsilon) + \dot{\lambda}(\varepsilon)\varepsilon Gx(\varepsilon). \end{aligned}$$

By setting ε equal to zero, it follows that

$$A\dot{x}(0) + Fx(0) = \lambda(0)B\dot{x}(0) + \dot{\lambda}(0)Bx(0) + \lambda(0)Gx(0).$$

Since $x(0) = x$ and $\lambda(0) = \lambda$ we have that

$$(A - \lambda B)\dot{x}(0) + (F - \lambda G)x = \dot{\lambda}(0)Bx.$$

Multiplying with v^{T} leads to

$$v^{\mathrm{T}}(A - \lambda B)\dot{x}(0) + v^{\mathrm{T}}(F - \lambda G)\, x = \dot{\lambda}(0)v^{\mathrm{T}}Bx.$$

The definition of v implies that the factor in front of $\dot{x}(0)$ is equal to zero. It follows that

$$\dot{\lambda}(0) = \frac{v^{\mathrm{T}}(F - \lambda G)x}{v^{\mathrm{T}}Bx}.$$

Since

$$\lambda(\varepsilon) = \lambda(0) + \varepsilon\dot{\lambda}(0) + \mathcal{O}(\varepsilon^2),$$

we may conclude that

$$\lambda(\varepsilon) - \lambda = \frac{v^{\mathrm{T}}(\varepsilon F - \lambda\varepsilon G)x}{v^{\mathrm{T}}Bx} + \mathcal{O}(\varepsilon^2).$$

3. An error estimate

Let us now apply this perturbation result to derive an error estimate. We recall that the Hankel matrices $\hat{H}_n(P_N)$ and $\hat{H}_n^<(P_N)$ have been previously defined as follows:

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

In [5] we have proved the following result.

Theorem 1. *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*

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

Define $\varphi_n(z)$ as the monic polynomial of degree n

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

and let

$$q_l(z) =: \frac{\varphi_n(z)}{\varphi_n'(z_l)(z - z_l)} := \sum_{k=0}^{n-1} q_{k,l}z^k,$$

for $l = 1,\ldots,n$. Note that $q_l(z)$ is a polynomial of degree $n-1$ and that $q_l(z_j) = \delta_{l,j}$ for $l,j = 1,\ldots,n$. The polynomials $q_1(z),\ldots,q_n(z)$ are linearly independent. Define the stacking vector $\vec{q_l}$ as

$$\vec{q_l} := \begin{bmatrix} q_{0,l} \\ q_{1,l} \\ \vdots \\ q_{n-1,l} \end{bmatrix}$$

for $l = 1,\ldots,n$.

Theorem 2. *The following holds*:

$$\hat{H}_n^{<}(P_N)\vec{q_l} = z_l \hat{H}_n(P_N)\vec{q_l} \quad \text{for } l = 1,\ldots,n.$$

In other words, $\vec{q_l}$ *is the right eigenvector corresponding to the eigenvalue* z_l.

Proof. Let $l \in \{1,\ldots,n\}$ and $k \in \{0,1,\ldots,n-1\}$. The $(k+1)$st element of the matrix–vector product $\hat{H}_n(P_N)\vec{q_l}$ is given by

$$\sum_{j=0}^{n-1} \hat{\mu}_{k+j}(P_N) q_{j,l}.$$

Theorem 1 implies that this sum is equal to

$$\sum_{j=0}^{n-1}\sum_{r=1}^{n} \frac{v_r}{1-z_r^K} z_r^{k+j} q_{j,l} = \sum_{r=1}^{n} \frac{v_r}{1-z_r^K} z_r^k \underbrace{\sum_{j=0}^{n-1} q_{j,l}\, z_r^j}_{=q_l(z_r)=\delta_{l,r}} = \frac{v_l z_l^k}{1-z_l^K}.$$

It follows that

$$\hat{H}_n(P_N)\vec{q_l} = \frac{v_l}{1-z_l^K} \begin{bmatrix} 1 \\ z_l \\ \vdots \\ z_l^{n-1} \end{bmatrix} =: \frac{v_l}{1-z_l^K}\vec{z_l}. \tag{2}$$

In an analogous way one can obtain

$$\hat{H}_n^{<}(P_N)\vec{q_l} = \frac{v_l z_l}{1-z_l^K}\vec{z_l}.$$

The theorem immediately follows from these two equations. □

Note that Eq. (2) implies that the matrix $\hat{H}_n(P_N)$ is nonsingular. Indeed, the following factorization is easily obtained:

$$\hat{H}_n^{<}(P_N) = \operatorname{diag}\left(\frac{v_1}{1-z_1^K},\ldots,\frac{v_n}{1-z_n^K}\right) [\vec{z_1} \quad \cdots \quad \vec{z_n}]\ [\vec{q_1} \quad \cdots \quad \vec{q_n}]^{-1}.$$

The matrix $[\vec{q_1} \ \cdots \ \vec{q_n}]$ is nonsingular as the polynomials $q_1(z),\ldots,q_n(z)$ are linearly independent. The diagonal matrix is nonsingular as the multiplicities are different from zero and the zeros $z_1,\ldots,z_n$ do not lie on the unit circle. Finally, the Vandermonde matrix $[\vec{z_1} \cdots \vec{z_n}]$ is nonsingular as the zeros are mutually distinct. It follows that $\hat{H}_n(P_N)$ is indeed nonsingular.

Let us now move on to the generalized eigenvalue problem involving f instead of (only) P_N. The matrices $\hat{H}_n(f), \hat{H}_n^{<}(f), \hat{H}_n(g)$ and $\hat{H}_n^{<}(g)$ are defined in a similar way as in (1). Let $\hat{z}_1,\ldots,\hat{z}_n$ denote the eigenvalues of the pencil $\hat{H}_n^{<}(f) - \lambda \hat{H}_n(f)$. Since

$$\hat{H}_n^{<}(f) = \hat{H}_n^{<}(P_N) + \hat{H}_n^{<}(g) \quad \text{and} \quad \hat{H}_n(f) = \hat{H}_n(P_N) + \hat{H}_n(g),$$

we can apply the perturbation result of Section 2. It follows that

$$\hat{z}_l - z_l = \frac{\vec{q_l}^{\mathrm{T}}(\hat{H}_n^{<}(g) - z_l \hat{H}_n(g))\vec{q_l}}{\vec{q_l}^{\mathrm{T}}\hat{H}_n(P_N)\vec{q_l}} + \mathcal{O}(\varepsilon^2),$$

for $l = 1, \ldots, n$, where ε is given by

$$\varepsilon = \max_{0 \leqslant k \leqslant 2n-1} |\hat{\mu}_k(g)|.$$

Let us analyse this expression in more detail. We start by considering the denominator. Eq. (2) immediately implies that

$$\vec{q_l}^{\mathrm{T}}\hat{H}_n(P_N)\vec{q_l} = \frac{v_l}{1 - z_l^K}\,\vec{q_l}^{\mathrm{T}}\vec{z_l} = \frac{v_l}{1 - z_l^K}\,q_l(z_l) = \frac{v_l}{1 - z_l^K}.$$

Next we turn our attention to the numerator. The following holds:

$$\begin{aligned}\vec{q_l}^{\mathrm{T}}\hat{H}_n(g)\vec{q_l} &= \sum_{i,j=0}^{n-1} q_{i,l}\,\hat{\mu}_{i+j}(g) q_{j,l}\\ &= \sum_{k=0}^{2n-2} \hat{\mu}_k(g) \sum_{\substack{i,j=0\\ i+j=k}}^{n-1} q_{i,l}q_{j,l}\\ &= \sum_{k=0}^{2n-2} q''_{k,l}\hat{\mu}_k(g)\end{aligned}$$

where the coefficients $q''_{k,l}$ are defined via

$$[q_l(z)]^2 =: \sum_{k=0}^{2n-2} q''_{k,l} z^k.$$

Since (cf. Eq. (7) in [5])

$$|\hat{\mu}_k(g)| \leqslant \sum_{r=1}^{+\infty} \frac{M}{\rho^{rK-k-1}} = M\frac{\left(\frac{1}{\rho}\right)^{K-k-1}}{1 - \left(\frac{1}{\rho}\right)^{K}},$$

it follows that

$$\begin{aligned}|\vec{q_l}^{\mathrm{T}}\hat{H}_n(g)\vec{q_l}| &\leqslant \frac{M}{1 - \rho^{-K}} \sum_{k=0}^{2n-2} |q''_{k,l}|\rho^{-K+k+1}\\ &= \frac{M\rho}{\rho^K - 1} \sum_{k=0}^{2n-2} |q''_{k,l}|\rho^{k}.\end{aligned}$$

In a similar way one can obtain that

$$\vec{q}_l^{\,\mathrm{T}} \hat{H}_n^{<}(g)\vec{q}_l = \sum_{k=0}^{2n-2} q''_{k,l}\hat{\mu}_{k+1}(g),$$

and that

$$|\vec{q}_l^{\,\mathrm{T}} \hat{H}_n^{<}(g)\vec{q}_l| \leqslant \frac{M\rho^2}{\rho^K - 1}\sum_{k=0}^{2n-2} |q''_{k,l}|\rho^k.$$

By combining these results we finally obtain that

$$|\hat{z}_l - z_l| \leqslant \frac{M}{v_l}\,|1 - z_l^K|\,\frac{\rho(\rho + |z_l|)}{\rho^K - 1}\sum_{k=0}^{2n-2} |q''_{k,l}|\rho^k + \mathcal{O}(\varepsilon^2)$$

for $l = 1, \ldots, n$, where $\varepsilon = \rho^{2n-K}$. Note that the first term on the right-hand side is (indeed) $\mathcal{O}(\rho^{2-K+2n-2} = \rho^{2n-K})$.

4. Numerical experiments

Let us illustrate this result with some numerical experiments.

Define

$$\eta_\rho(z_l) := \frac{M}{v_l}|1 - z_l^K|\frac{\rho(\rho + |z_l|)}{\rho^K - 1}\sum_{k=0}^{2n-2}|q''_{k,l}|\rho^k$$

for $l = 1, \ldots, n$, then $|\hat{z}_l - z_l| \leqslant \eta_\rho(z_l) + \mathcal{O}(\varepsilon^2), \quad l = 1, \ldots, n.$

In the following examples, the calculations have been carried out by using Mathematica in multiple precision arithmetic (about 64 decimal digits). The constant

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

has been approximated by

$$\max_{0 \leqslant j \leqslant \hat{K}-1}\left\{\left|\frac{g'(\rho\hat{\omega}_j)}{g(\rho\hat{\omega}_j)}\right|\right\}$$

where $\hat{K}$ and $\hat{\omega}_j := \exp(2\pi ij/\hat{K})$ for $j = 0, 1, \ldots, \hat{K} - 1$.

Suppose that $N = 6$ and let

$$P_N(z) = (z - 0.2 + 0.5i)(z - 0.2 - 0.5i)(z - 0.2)(z - 0.21)(z + 0.95)^2$$

and

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

Table 1
Absolute approximation errors for various values of $K (\rho = 1.9)$

	$\lvert\hat{z}_l - z_l\rvert$			
z_l	$K = 40$	$K = 48$	$K = 56$	$K = 64$
$0.5 + 0.2i$	5.45e-09	2.13e-11	8.31e-14	3.25e-16
$0.5 - 0.2i$	5.45e-09	2.13e-11	8.31e-14	3.25e-16
0.2	6.77e-05	2.63e-07	1.03e-09	4.01e-12
0.21	6.60e-05	2.59e-07	1.01e-09	3.96e-12
-0.95	2.24e-11	9.18e-14	3.70e-16	1.47e-18

Table 2
Corresponding error bounds $(\rho = 1.9)$

	$\eta_\rho(\hat{z}_l)$			
z_l	$K = 40$	$K = 48$	$K = 56$	$K = 64$
$0.5 + 0.2i$	2.07e-05	1.22e-07	7.19e-10	4.23e-12
$0.5 - 0.2i$	2.07e-05	1.22e-07	7.19e-10	4.23e-12
0.2	1.52e-01	8.82e-04	5.19e-06	3.05e-08
0.21	1.46e-01	8.74e-04	5.14e-06	3.03e-08
-0.95	1.83e-07	1.13e-09	6.86e-12	4.11e-14

Table 3
Absolute approximation errors and error bounds for various values of $\rho (K = 64)$

		$\eta_\rho(\hat{z}_l)$			
z_l	$\lvert\hat{z}_l - z_l\rvert$	$\rho = 1.99$	$\rho = 1.90$	$\rho = 1.80$	$\rho = 1.60$
$0.5 + 0.2i$	3.2e-16	3.8e-13	4.2e-12	7.0e-11	3.3e-08
$0.5 - 0.2i$	3.2e-16	3.8e-13	4.2e-12	7.0e-11	3.3e-08
0.2	4.0e-12	2.8e-09	3.0e-08	4.9e-07	2.2e-04
0.21	4.0e-12	2.8e-09	3.0e-08	4.9e-07	2.2e-04
-0.95	1.5e-18	3.7e-15	4.1e-14	6.9e-13	3.3e-10

observe that $\rho < 2$. In our first numerical experiment, we set $\rho = 1.9$. Table 1 lists the absolute approximation errors for various values of (the number of quadrature points) K. Table 2 shows the corresponding values of η_ρ, the first-order term of our error bound, which in this specific example turns out to be rather conservative. Next, we consider various values of ρ. Table 3 lists the results. As is to be expected, the sharper the ρ, the better is the error bound. The error bounds for the zeros 0.2 and 0.21 show that these zeros are rather ill-conditioned.

To evaluate the error bound η_ρ, one needs z_l, $l = 1, \ldots, n$, as well as $g(z)$, which limits the applicability of η_ρ to theoretical considerations. We will now show how to use the approximate

Table 4
Error bounds based on $\hat{z}_l$ for various values of $K(\rho = 1.9)$

	$\hat{\eta}_\rho(\hat{z}_l)$			
z_l	$K = 40$	$K = 48$	$K = 56$	$K = 64$
$0.5 + 0.2i$	2.07e-05	1.22e-07	7.17e-10	4.22e-12
$0.5 - 0.2i$	2.07e-05	1.22e-07	7.17e-10	4.22e-12
0.2	1.49e-01	8.79e-04	5.18e-06	3.05e-08
0.21	1.48e-01	8.71e-04	5.13e-06	3.02e-08
-0.95	1.82e-07	1.13e-09	6.84e-12	4.11e-14

zeros $\hat{z}_l$ instead of the zeros z_l themselves. Let

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

and let

$$\hat{q}_l(z) := \frac{\hat{\varphi}_n(z)}{\hat{\varphi}_n'(\hat{z}_l)(z - \hat{z}_l)}$$

for $l = 1, \ldots, n$. Let the coefficients $\hat{q}''_{k,l}$ be defined by

$$[\hat{q}_l(z)]^2 =: \sum_{k=0}^{2n-2} \hat{q}''_{k,l} z^k.$$

Let $\hat{v}_1, \ldots, \hat{v}_n$ be the solutions of the linear system of equations

$$\sum_{k=1}^{n} \left(\frac{\hat{z}_k^p}{1 - \hat{z}_k^K} \right) \hat{v}_k = \hat{\mu}_p(f), \quad p = 0, \ldots, n-1.$$

Define

$$\hat{M} := \max_{0 \leqslant j \leqslant \hat{K}-1} \left\{ \left| \frac{f'(\rho\hat{\omega}_j)}{f(\rho\hat{\omega}_j)} - \sum_{l=1}^{n} \frac{\hat{v}_l}{\rho\hat{\omega}_j - \hat{z}_l} \right| \right\}, \tag{3}$$

then the new error bound is given by

$$\hat{\eta}_\rho(\hat{z}_l) := \frac{\hat{M}}{\hat{v}_l} |1 - \hat{z}_l^K| \frac{\rho(\rho + |\hat{z}_l|)}{\rho^K - 1} \sum_{k=0}^{2n-2} |\hat{q}''_{k,l}| \rho^k \tag{4}$$

for $l = 1, \ldots, n$. Table 4 lists the numerical results. They are very similar to those given in Table 2.

5. Generalizations

Let us briefly suggest a few generalizations that could be interesting topics for further consideration. The present paper concerns only a circular region and the trapezoidal quadrature rule along the circumference of the circle. Other possibilities may concern the study of poles of meromorphic functions (not only zeros of analytic functions, cf. the paper [4]), the study of more general regions (such as an ellipse, a square or, preferably, an arbitrary finite region), the study of infinite regions (e.g., the region outside the unit circle), the study of the whole plane for an analytic function with a discontinuity interval (e.g., the interval $[-1, 1]$), i.e., a sectionally analytic function, etc. We hope to address these cases, including an error analysis, in future publications.

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