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via modified moments based on  
formal orthogonal polynomials**

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*Report TW 246, November 1996*



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## **Abstract**

We consider the problem of computing all the zeros of an analytic function that lie in the interior of a Jordan curve, together with their respective multiplicities. Our approach uses modified moments based on formal orthogonal polynomials. Numerical experiments indicate that it is far superior to classical approaches, which consider the usually ill-conditioned map from the Newton sums to the unknowns.

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# COMPUTING ZEROS OF ANALYTIC FUNCTIONS VIA MODIFIED MOMENTS BASED ON FORMAL ORTHOGONAL POLYNOMIALS

PETER KRAVANJA, MARC VAN BAREL, AND ANN HAEGEMANS

ABSTRACT. We consider the problem of computing all the zeros of an analytic function that lie in the interior of a Jordan curve, together with their respective multiplicities. Our approach uses modified moments based on formal orthogonal polynomials. Numerical experiments indicate that it is far superior to classical approaches, which consider the usually ill-conditioned map from the Newton sums to the unknowns.

## 1. INTRODUCTION

Let  $W$  be a simply connected region in  $\mathbb{C}$ ,  $f : W \rightarrow \mathbb{C}$  analytic in  $W$ , and  $\gamma$  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  $\gamma$ , together with their respective multiplicities.

Let  $N$  denote the total number of zeros of  $f$  that lie in the interior of  $\gamma$ , i.e., the number of zeros where each zero is counted according to its multiplicity. Suppose that  $N > 0$ . Let  $n$  be the number of mutually distinct zeros of  $f$  that lie in the interior of  $\gamma$ . Let  $z_1, \dots, z_n$  be these zeros and  $\nu_1, \dots, \nu_n$  their respective multiplicities. An easy calculation shows that  $z_k$  is a simple pole of  $f'/f$  with residue  $\nu_k$  for  $k = 1, \dots, n$ . 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. 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 [10]. A classical approach is to consider the integrals

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

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

$$s_p = \sum_{k=1}^n \nu_k z_k^p, \quad p = 0, 1, 2, \dots,$$

and thus the problem is transformed into that of solving a system of polynomial equations. This approach has been taken by Delves and Lyness [3] and was reconsidered by Li [12] and, recently, by the authors [11]. Let us recall the results obtained in [11]. Define  $H$  as the infinite Hankel matrix

$$H := [s_{p+q}]_{p,q \geq 0}$$

and let

$$H_k := \begin{bmatrix} s_0 & s_1 & \cdots & s_{k-1} \\ s_1 & & \ddots & \vdots \\ \vdots & \ddots & & \vdots \\ s_{k-1} & \cdots & \cdots & s_{2k-2} \end{bmatrix}, \quad k = 1, 2, \dots,$$

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be its  $k \times k$  leading principal submatrix. Define also the  $k \times k$  matrix  $H_k^<$  as

$$H_k^< := \begin{bmatrix} s_1 & s_2 & \cdots & s_k \\ s_2 & & \ddots & \vdots \\ \vdots & \ddots & & \vdots \\ s_k & \cdots & \cdots & s_{2k-1} \end{bmatrix}, \quad k = 1, 2, \dots$$

In what follows we will assume that all the  $s_p$ 's that are needed have been calculated (via numerical integration). In particular, we will assume that the value of  $N$  is known. Then  $n$  can be calculated as  $\text{rank } H_N$ .

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

Once  $n$  is known, the zeros  $z_1, \dots, z_n$  can be calculated by solving a generalized eigenvalue problem that has Hankel structure.

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

Once  $z_1, \dots, z_n$  have been found, the multiplicities  $\nu_1, \dots, \nu_n$  can be computed by solving the Vandermonde system

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

Theoretically the  $N - n$  smallest singular values of  $H_N$  are equal to zero. In practice, this will not be the case, as by evaluating the corresponding integrals numerically one can only obtain approximations for the  $s_p$ 's and because of roundoff errors in the SVD computation. If the numerical rank  $n$  of  $H_N$  is difficult to determine, it is safe to consider  $H_N$  as a matrix of full rank and to solve an  $N \times N$  generalized eigenvalue problem and associated Vandermonde system.

**Theorem 3.** For every integer  $t \geq n$  the eigenvalues of the pencil  $H_t^< - \lambda H_t$  are given by  $z_1, \dots, z_n$  and  $t - n$  eigenvalues that may assume arbitrary values.

Each of these  $t - n$  indeterminate eigenvalues corresponds to two corresponding zeros on the diagonals of the generalized Schur decomposition of  $H_t^<$  and  $H_t$ . When actually calculated, these diagonal entries are different from zero because of roundoff errors. The quotient of two such corresponding diagonal entries is an eigenvalue that is not a zero of  $f$ . Fortunately, the corresponding Vandermonde system enables one to detect such spurious "zeros." Indeed, its matrix will almost surely (i.e., with probability one) be regular and therefore the system will have only one solution, which gives the true zeros of  $f$  their correct corresponding multiplicity and the spurious ones "multiplicity" zero.

Unfortunately, the map from the Newton sums to the zeros and their respective multiplicities is usually ill-conditioned (see [11] and also the papers of Gautschi [6, 7] who studied the conditioning of this map in the context of Gauss quadrature formulae). Suppose for example that  $n = 6$ ,

$$z_1 = 1, \quad z_2 = 2, \quad z_3 = 3, \quad z_4 = 4, \quad z_5 = 5, \quad z_6 = 6$$

and  $\nu_1 = \dots = \nu_6 = 1$ . Then by computing the Newton sums explicitly as  $s_p = \sum_{k=1}^n \nu_k z_k^p$  and by calculating the eigenvalues of  $H_n^< - \lambda H_n$  using Matlab (with floating point relative accuracy  $\approx 2.2204 \cdot 10^{-16}$ ), we obtain

$$\begin{array}{lll} 1.000000000007227, & 2.000000000339424, & 3.000000002071328, \\ 4.000000002666899, & 5.000000000762610, & 6.000000000031502. \end{array}$$

(The imaginary parts are not shown—they are  $\mathcal{O}(10^{-12})$ .) The conditioning is particularly bad in the case of clustered zeros. For example, if  $n = 6$ ,

$$\begin{array}{lll} z_1 = 3, & z_2 = 3.00001, & z_3 = 3.00002, \\ z_4 = 8, & z_5 = 8.00002, & z_6 = 8 + i 0.00001 \end{array}$$

and  $\nu_1 = \dots = \nu_6 = 1$ , then we would obtain

$$\begin{aligned} -8.929298009058625 + i 0.000131585717976, & \quad 3.000009996398890 + i 0.000000000000279, \\ 3.018824719310254 - i 0.000004739453523, & \quad 5.539985015441636 + i 0.001639228103641, \\ 8.000006673486054 + i 0.000003317117220, & \quad 7.996191856990388 - i 0.002550799354460. \end{aligned}$$

In [11] we have reduced the ill-conditioning by first shifting the origin in the complex plane to the arithmetic mean of the zeros,

$$\mu := \frac{\sum_{k=1}^n \nu_k z_k}{\sum_{k=1}^n \nu_k} = \frac{s_1}{s_0}.$$

Then the zeros are better relatively separated, which is appropriate in floating point arithmetic, as we argued intuitively. In this approach the unknowns are calculated from the integrals

$$\frac{1}{2\pi i} \int_{\gamma} (z - \mu)^p \frac{f'(z)}{f(z)} dz, \quad p = 0, 1, 2, \dots,$$

i.e., by using the shifted monomial basis  $\{(z - \mu)^k\}_{k \geq 0}$  instead of the standard basis  $\{z^k\}_{k \geq 0}$ . In this paper we will show how  $n, z_1, \dots, z_n$  and  $\nu_1, \dots, \nu_n$  can be calculated from integrals involving an arbitrary polynomial basis  $\{\psi_k(z)\}_{k \geq 0}$ . By analogy with numerical quadrature, we call this an approach based on *modified moments*. The formal orthogonal polynomials associated with the measure that puts mass  $\nu_k$  at  $z_k$  for  $k = 1, \dots, n$  will turn out to be excellent choices for the  $\psi_k$ 's. By applying the algorithm explained in Section 3 to the previous examples, we obtain

$$\begin{aligned} 1.000000000000001, & \quad 2.000000000000000, \\ 3.000000000000000, & \quad 4.000000000000000, \\ 5.000000000000000, & \quad 6.000000000000001 \end{aligned}$$

and

$$\begin{aligned} 2.99999999735130 - i 0.00000000001420, & \quad 3.000009998575106 + i 0.00000000058456, \\ 3.000019999736600 + i 0.00000000000931, & \quad 7.999999992384290 + i 0.000000088570409, \\ 8.000020157615410 + i 0.000000017110382, & \quad 7.999999851862055 + i 0.000009892258188. \end{aligned}$$

This paper is organized as follows. In Section 2 we discuss the properties of formal orthogonal polynomials that are relevant to our purpose. In Section 3 we explain how to use modified moments and we formulate our algorithm. We conclude with numerical examples in Section 4.

## 2. FORMAL ORTHOGONAL POLYNOMIALS

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

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

by setting

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

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

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

$$(2) \quad \langle z^k, \varphi_t(z) \rangle = 0, \quad k = 0, 1, \dots, t-1,$$

is called a *formal orthogonal polynomial* (FOP) of degree  $t$ . (Note that condition (2) is void for  $t = 0$ .) The adjective *formal* emphasizes the fact that, in general, the bilinear form (1) 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  $\varphi_t$  need not exist or need not be unique for every degree  $t$ . (For details, see [9] and the references cited therein.) If (2) is satisfied and  $\varphi_t$  is unique, then  $\varphi_t$  is called a *regular* FOP and  $t$  a *regular index*. If we set

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

then condition (2) translates into the *Yule-Walker* system

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

Hence, the regular FOP of degree  $t \geq 1$  exists if and only if the matrix  $H_t$  is regular. Thus, the rank profile of  $H$  determines which regular FOPs exist. If  $t$  is a regular index, then

$$(4) \quad \varphi_t(z) = \frac{1}{\det H_t} \begin{vmatrix} s_0 & s_1 & \cdots & s_{t-1} & 1 \\ s_1 & & \ddots & \vdots & z \\ \vdots & \ddots & & \vdots & \vdots \\ s_{t-1} & \cdots & \cdots & s_{2t-2} & z^{t-1} \\ s_t & \cdots & \cdots & s_{2t-1} & z^t \end{vmatrix},$$

as one can easily verify. Note that this implies that

$$\langle \varphi_t, \varphi_t \rangle = \frac{\det H_{t+1}}{\det H_t}.$$

The regular FOP of degree 1 exists and is given by  $\varphi_1(z) = z - \mu$  where  $\mu = s_1/s_0$  is the arithmetic mean of the zeros. Theorem 1 implies that the regular FOP  $\varphi_n$  of degree  $n$  exists and tells us also that regular FOPs of degree larger than  $n$  do not exist. The polynomial  $\varphi_n$  is easily seen to be

$$\varphi_n(z) = (z - z_1) \cdots (z - z_n).$$

It is the monic polynomial of degree  $n$  that has  $z_1, \dots, z_n$  as simple zeros. Its coefficients can be calculated by solving an  $n \times n$  Yule-Walker system. This polynomial has the peculiar property that it is orthogonal to *all* polynomials (including itself),

$$\langle z^k, \varphi_n(z) \rangle = 0, \quad k = 0, 1, 2, \dots$$

(In fact, the orthogonal complement  $\mathcal{P}^\perp$  of  $\mathcal{P}$  in  $\mathcal{P}$  is an ideal generated by  $\varphi_n$ .) Theorem 2 can now be interpreted as follows: the zeros of the regular FOP of degree  $n$  are given by the eigenvalues of the pencil  $H_n^< - \lambda H_n$ . The following theorem shows that this zero/eigenvalue property holds for all regular FOPs.

**Theorem 4.** *Let  $t \geq 1$  be a regular index. Then the zeros of the regular FOP  $\varphi_t$  of degree  $t$  are given by the eigenvalues of the pencil  $H_t^< - \lambda H_t$ .*

*Proof.* Suppose  $\varphi_t(z) =: u_{0,t} + u_{1,t}z + \cdots + u_{t-1,t}z^{t-1} + z^t$ . Then the zeros of  $\varphi_t$  are given by the eigenvalues of its companion matrix

$$C_t := \begin{bmatrix} 0 & 0 & \cdots & 0 & -u_{0,t} \\ 1 & 0 & \cdots & 0 & -u_{1,t} \\ 0 & 1 & \ddots & \vdots & \vdots \\ \vdots & & \ddots & 0 & -u_{t-2,t} \\ 0 & \cdots & 0 & 1 & -u_{t-1,t} \end{bmatrix}.$$

Let  $\lambda$  be an eigenvalue of  $C_t$  and  $x$  a corresponding eigenvector. As  $H_t$  is regular, we may conclude that

$$C_t x = \lambda x \Leftrightarrow H_t C_t x = \lambda H_t x.$$

Using (3) one can easily verify that  $H_t C_t = H_t^<$ . This proves the theorem.  $\square$

If  $H_n$  is strongly regular, i.e., if all its leading principal submatrices are regular, then we have a full set  $\{\varphi_0, \varphi_1, \dots, \varphi_n\}$  of regular FOPs. Note that in this case the  $n \times n$  Gram matrix  $G_n := [\langle \varphi_p, \varphi_q \rangle]_{p,q=0}^{n-1}$  is diagonal, and that the matrix  $G_n^{(1)} := [\langle \varphi_p, \varphi_1 \varphi_q \rangle]_{p,q=0}^{n-1}$  is tridiagonal.

What happens if  $H_n$  is not strongly regular and thus there is no full set of regular FOPs? Let  $\{k_j\}_{j=0}^J$  be the set of all regular indices, with

$$k_0 < k_1 < \dots < k_J.$$

Then  $k_0 = 0$ ,  $k_1 = 1$  and  $k_J = n$ . 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  $\varphi_t$  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 (1). More precisely, define  $\{\varphi_t\}_{t=0}^\infty$  as follows. If  $t$  is a regular index, then let  $\varphi_t$  be the regular FOP of degree  $t$ . Else define  $\varphi_t$  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  $\varphi_t$  is called an *inner polynomial*. If  $\psi_{t,r}(z) = z^{t-r}$  then we say that  $\varphi_t$  is defined *by using the standard monomial basis*. These polynomials  $\{\varphi_t\}_{t=0}^\infty$  can be grouped into  $J + 1$  blocks

$$\begin{aligned} \Phi^{(0)} &:= [\varphi_0] \\ \Phi^{(1)} &:= [\varphi_1 \quad \varphi_2 \quad \dots \quad \varphi_{k_2-1}] \\ \Phi^{(2)} &:= [\varphi_{k_2} \quad \varphi_{k_2+1} \quad \dots \quad \varphi_{k_3-1}] \\ &\vdots \\ \Phi^{(J-1)} &:= [\varphi_{k_{J-1}} \quad \varphi_{k_{J-1}+1} \quad \dots \quad \varphi_{k_J-1}] \\ \Phi^{(J)} &:= [\varphi_n \quad \varphi_{n+1} \quad \dots]. \end{aligned}$$

Note that each block starts with a regular FOP and that the remaining polynomials in each block are inner polynomials. The  $p$ th block has length  $l_p := k_{p+1} - k_p$  for  $p = 0, 1, \dots, J - 1$ . Let

$$\langle \Psi, \Phi \rangle := \begin{bmatrix} \langle \psi_0, \phi_0 \rangle & \dots & \langle \psi_0, \phi_q \rangle \\ \vdots & & \vdots \\ \langle \psi_p, \phi_0 \rangle & \dots & \langle \psi_p, \phi_q \rangle \end{bmatrix} \in \mathbb{C}^{(p+1) \times (q+1)}$$

for any two row vectors

$$\Psi := [\psi_0 \quad \psi_1 \quad \dots \quad \psi_p] \quad \text{and} \quad \Phi := [\phi_0 \quad \phi_1 \quad \dots \quad \phi_q]$$

of polynomials in  $\mathcal{P}$ .

**Theorem 5.** *The following block orthogonality relations hold:*

$$\langle \Phi^{(p)}, \Phi^{(q)} \rangle = \begin{cases} 0_{l_p \times l_q} & \text{if } p \neq q \\ \delta_p & \text{if } p = q \end{cases} \quad \text{for } p, q = 0, 1, \dots, J - 1$$

where the matrix  $\delta_p \in \mathbb{C}^{l_p \times l_p}$  is regular, symmetric, zero above the main antidiagonal and equal to  $\langle z^{k_p+l_p-1}, \varphi_{k_p} \rangle$  along the main antidiagonal for  $p = 0, 1, \dots, J - 1$ . Also, if all the inner polynomials of the block  $\Phi^{(p)}$  where  $p \in \{1, \dots, J - 1\}$  are defined by using the standard monomial basis, then  $\delta_p$  is a Hankel matrix.

*Proof.* The proof is by induction. Obviously,  $\langle \Phi^{(0)}, \Phi^{(0)} \rangle = [\langle 1, 1 \rangle] = [s_0]$  is regular. Now suppose that the theorem holds for  $p, q = 0, 1, \dots, k - 1$  where  $k \in \{1, \dots, J - 1\}$ . Consider the block  $\Phi^{(k)}$ . Let us call the first polynomial of this block  $\varphi_r$  and let  $l$  be the length of this block,

$$\Phi^{(k)} = [\varphi_r \quad \varphi_{r+1} \quad \dots \quad \varphi_{r+l-1}].$$

Then the matrices  $H_{r+1}, \dots, H_{r+l-1}$  are singular while  $H_r$  and  $H_{r+l}$  are regular. By symmetry considerations it suffices to prove that

$$\hat{K} := \begin{bmatrix} \langle \varphi_0, \varphi_r \rangle & \dots & \langle \varphi_0, \varphi_{r+l-1} \rangle \\ \langle \varphi_1, \varphi_r \rangle & \dots & \langle \varphi_1, \varphi_{r+l-1} \rangle \\ \vdots & & \vdots \\ \langle \varphi_{r-1}, \varphi_r \rangle & \dots & \langle \varphi_{r-1}, \varphi_{r+l-1} \rangle \end{bmatrix} = 0_{r \times l}$$

and that the matrix

$$\hat{\delta} := \begin{bmatrix} \langle \varphi_r, \varphi_r \rangle & \cdots & \langle \varphi_r, \varphi_{r+l-1} \rangle \\ \vdots & & \vdots \\ \langle \varphi_{r+l-1}, \varphi_r \rangle & \cdots & \langle \varphi_{r+l-1}, \varphi_{r+l-1} \rangle \end{bmatrix}$$

is regular and has the other properties mentioned. Let  $F_l$  be the  $l \times l$  unit upper triangular matrix that contains the coefficients of the polynomials  $1, \psi_{r+1,r}, \dots, \psi_{r+l-1,r}$  (used in the definition of the inner polynomials of this block). Then

$$\hat{K} = KF_l \quad \text{and} \quad \hat{\delta} = F_l^T \delta F_l$$

if the matrices  $K$  and  $\delta$  are defined as

$$K := \begin{bmatrix} \langle \varphi_0, \varphi_r \rangle & \langle \varphi_0, z\varphi_r \rangle & \cdots & \langle \varphi_0, z^{l-1}\varphi_r \rangle \\ \vdots & \vdots & & \vdots \\ \langle \varphi_{r-1}, \varphi_r \rangle & \langle \varphi_{r-1}, z\varphi_r \rangle & \cdots & \langle \varphi_{r-1}, z^{l-1}\varphi_r \rangle \end{bmatrix}$$

and

$$\delta := \begin{bmatrix} \langle \varphi_r, \varphi_r \rangle & \langle \varphi_r, z\varphi_r \rangle & \cdots & \langle \varphi_r, z^{l-1}\varphi_r \rangle \\ \langle z\varphi_r, \varphi_r \rangle & & \cdots & \vdots \\ \vdots & \ddots & & \vdots \\ \langle z^{l-1}\varphi_r, \varphi_r \rangle & \cdots & \cdots & \langle z^{l-1}\varphi_r, z^{l-1}\varphi_r \rangle \end{bmatrix}.$$

(In other words,  $K$  and  $\delta$  correspond to the situation where all the inner polynomials in our block are defined by using the standard monomial basis.) Therefore we will first study the matrices  $K$  and  $\delta$ . Observe that  $\delta$  is a Hankel matrix. As  $\varphi_r$  is a regular FOP, we may conclude that  $\langle \varphi_s, z^t \varphi_r \rangle = 0$  for  $t \geq 0$  and  $s = 0, 1, \dots, r-t-1$ . Thus

$$(5) \quad K = \begin{bmatrix} 0 & \cdots & \cdots & 0 \\ \vdots & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ 0 & \cdots & \cdots & 0 \\ \vdots & & \ddots & \times \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \times & \cdots & \times \end{bmatrix}.$$

Let us consider the first antidiagonal of  $K$  whose entries we have not yet proven to be equal to zero. As  $\varphi_r$  is orthogonal to all polynomials of degree  $\leq r-1$ , all these entries are equal. Indeed,

$$\langle \varphi_{r-1}, z\varphi_r \rangle = \langle \varphi_{r-2}, z^2\varphi_r \rangle = \cdots = \langle \varphi_{r-l+1}, z^{l-1}\varphi_r \rangle = \langle z^r, \varphi_r \rangle.$$

Note that  $\langle z^r, \varphi_r \rangle = \langle \varphi_r, \varphi_r \rangle$ , the entry in the upper left corner of  $\delta$ . As  $H_{r+1}$  is singular and  $\langle \varphi_r, \varphi_r \rangle = \det H_{r+1} / \det H_r$ , it follows that  $\langle \varphi_r, \varphi_r \rangle = 0$ . This implies that  $\varphi_r$  is in fact orthogonal to all polynomials of degree  $\leq r$  and that the upper left entry of  $\delta$  as well as all the entries on our antidiagonal of  $K$  are equal to zero. Now we continue with the next antidiagonal of  $K$ . The fact that  $\langle \varphi_r, \varphi_r \rangle = 0$  implies that all its entries are equal to  $\langle z^{r+1}, \varphi_r \rangle = \langle z\varphi_r, \varphi_r \rangle$ . One can easily check that

$$R_{r+2}^T H_{r+2} R_{r+2} = [\langle \varphi_p, \varphi_q \rangle]_{p,q=0}^{r+1} = \text{diag}(\delta_0, \delta_1, \dots, \delta_{k-1}) \oplus F_2^T \begin{bmatrix} 0 & \langle z^{r+1}, \varphi_r \rangle \\ \langle z^{r+1}, \varphi_r \rangle & \langle z\varphi_r, z\varphi_r \rangle \end{bmatrix} F_2$$

if  $R_{r+2}$  is the unit upper triangular matrix that contains the coefficients of  $\varphi_0, \varphi_1, \dots, \varphi_{r+1}$ . As  $H_{r+2}$  is singular and  $\delta_0, \delta_1, \dots, \delta_{k-1}$  are regular, it follows that  $\langle z^{r+1}, \varphi_r \rangle = 0$ . Thus  $\varphi_r$  is orthogonal to all polynomials of degree  $\leq r+1$  and all the entries on our antidiagonal of  $K$  as well as two additional entries of  $\delta$  are equal to zero. And so on. Eventually we will find that all the entries of  $K$  that are marked  $\times$  in (5) are determined by the first  $l-1$  entries of the first row of  $\delta$  "in a Hankel way," i.e., by shifting these entries to the north-east. We will also find that  $\langle z^{r+2}, \varphi_r \rangle = \cdots = \langle z^{r+l-2}, \varphi_r \rangle = 0$ , i.e.,  $\varphi_r$  is orthogonal to all polynomials of





Note that  $M_k$  as well as  $M_k^{(1)}$  are symmetric for all  $k$ . In what follows we will assume that all the “inner products”  $\langle \psi_p, \psi_q \rangle$  and  $\langle \psi_p, \psi_1 \psi_q \rangle$  that are needed have been calculated.

As  $\langle \psi_r, \varphi_n \rangle = 0$  for  $r = 0, 1, 2, \dots$ , it follows immediately that the coefficients  $\sigma_1, \dots, \sigma_n$  in the expansion

$$\varphi_n(z) = \prod_{k=1}^n (z - z_k) =: \psi_n(z) + \sigma_1 \psi_{n-1}(z) + \dots + \sigma_n \psi_0(z)$$

can be computed by solving the linear system of equations

$$\begin{bmatrix} m_{0,0} & \cdots & m_{0,n-1} \\ \vdots & & \vdots \\ m_{n-1,0} & \cdots & m_{n-1,n-1} \end{bmatrix} \begin{bmatrix} \sigma_n \\ \vdots \\ \sigma_1 \end{bmatrix} = - \begin{bmatrix} m_{0,n} \\ \vdots \\ m_{n-1,n} \end{bmatrix}.$$

The matrix of this system is regular. Indeed, one can easily verify that  $M_n$  can be factorized as

$$M_n = V_n D_n V_n^T$$

where  $V_n$  is the Vandermonde-like matrix

$$V_n := \begin{bmatrix} \psi_0(z_1) & \cdots & \psi_0(z_n) \\ \vdots & & \vdots \\ \psi_{n-1}(z_1) & \cdots & \psi_{n-1}(z_n) \end{bmatrix}$$

and  $D_n := \text{diag}(\nu_1, \dots, \nu_n)$ . The following theorem generalizes Theorem 1.

**Theorem 9.**  $n = \text{rank } M_{n+p}$  for every integer  $p \geq 0$ . In particular,  $n = \text{rank } M_N$ .

*Proof.* This follows immediately from Theorem 1 and the fact that  $M_t$  can be factorized for every  $t \geq 1$  as  $M_t = A_t^T H_t A_t$  if  $A_t$  is the unit upper triangular matrix that contains the coefficients of  $\psi_0, \psi_1, \dots, \psi_{t-1}$ . Another, more direct proof is the following. Let  $p$  be a nonnegative integer. The matrix  $M_{n+p}$  can be written as

$$\begin{aligned} M_{n+p} &= \sum_{k=1}^n \nu_k \begin{bmatrix} \psi_0(z_k) \psi_0(z_k) & \cdots & \psi_0(z_k) \psi_{n+p-1}(z_k) \\ \vdots & & \vdots \\ \psi_{n+p-1}(z_k) \psi_0(z_k) & \cdots & \psi_{n+p-1}(z_k) \psi_{n+p-1}(z_k) \end{bmatrix} \\ &= \sum_{k=1}^n \nu_k \begin{bmatrix} \psi_0(z_k) \\ \vdots \\ \psi_{n+p-1}(z_k) \end{bmatrix} [\psi_0(z_k) \cdots \psi_{n+p-1}(z_k)]. \end{aligned}$$

This implies that  $\text{rank } M_{n+p} \leq n$ . However,  $M_n$  is regular and thus  $\text{rank } M_{n+p} \geq n$ . It follows that  $\text{rank } M_{n+p} = n$ .  $\square$

**Theorem 10.** Let  $t$  be a positive integer. Then  $\lambda^*$  is an eigenvalue of the pencil  $H_t^< - \lambda H_t$  if and only if  $\psi_1(\lambda^*)$  is an eigenvalue of the pencil  $M_t^{(1)} - \lambda M_t$ .

*Proof.* Let  $A_t$  be the unit upper triangular matrix that contains the coefficients of  $\psi_0, \psi_1, \dots, \psi_{t-1}$ . Then  $M_t$  can be factorized as  $M_t = A_t^T H_t A_t$ . Suppose  $\psi_1(z) =: z - \beta$ . Then  $M_t^{(1)}$  is given by  $[\langle \psi_p, z \psi_q \rangle]_{p,q=0}^{t-1} - \beta M_t$ . The matrix  $[\langle \psi_p, z \psi_q \rangle]_{p,q=0}^{t-1}$  can be written as  $A_t^T H_t^< A_t$  and thus  $M_t^{(1)} = A_t^T (H_t^< - \beta H_t) A_t$ . Now let  $\lambda^*$  be an eigenvalue of the pencil  $H_t^< - \lambda H_t$  and  $x$  a corresponding eigenvector. Then

$$\begin{aligned} &H_t^< x = \lambda^* H_t x \\ \Leftrightarrow &(H_t^< - \beta H_t) x = (\lambda^* - \beta) H_t x \\ \Leftrightarrow &A_t^T (H_t^< - \beta H_t) A_t y = \psi_1(\lambda^*) A_t^T H_t A_t y \quad \text{if } y := A_t^{-1} x. \\ \Leftrightarrow &M_t^{(1)} y = \psi_1(\lambda^*) M_t y. \end{aligned}$$

This proves the theorem.  $\square$

**Corollary 11.** *Let  $t \geq 1$  be a regular index and let  $z_{t,1}, \dots, z_{t,t}$  be the zeros of the regular FOP  $\varphi_t$ . Then the eigenvalues of the pencil  $G_t^{(1)} - \lambda G_t$  are given by  $z_{t,1} - \mu, \dots, z_{t,t} - \mu$  where  $\mu = s_1/s_0$  is the arithmetic mean of the zeros. In particular, the eigenvalues of the pencil  $G_n^{(1)} - \lambda G_n$  are given by  $z_1 - \mu, \dots, z_n - \mu$ .*

Once the zeros  $z_1, \dots, z_n$  have been calculated, their respective multiplicities can be computed by solving the Vandermonde-like system

$$(6) \quad \begin{bmatrix} \psi_0(z_1) & \cdots & \psi_0(z_n) \\ \vdots & & \vdots \\ \psi_{n-1}(z_1) & \cdots & \psi_{n-1}(z_n) \end{bmatrix} \begin{bmatrix} \nu_1 \\ \vdots \\ \nu_n \end{bmatrix} = \begin{bmatrix} m_{0,0} \\ \vdots \\ m_{n-1,0} \end{bmatrix}.$$

**Special cases.** Let us consider a few special cases. Suppose that the polynomials  $\psi_k$  satisfy a three-term recurrence relation,

$$\psi_{-1}(z) := 0, \quad \psi_0(z) = 1$$

and

$$\psi_k(z) = (z - \alpha_k)\psi_{k-1}(z) + \beta_k\psi_{k-2}(z)$$

for  $k = 1, 2, \dots$  with  $\beta_1 := 0$ . As

$$\begin{aligned} \psi_1(z)\psi_q(z) &= (z - \alpha_1)\psi_q(z) \\ &= (z - \alpha_{q+1})\psi_q(z) + (\alpha_{q+1} - \alpha_1)\psi_q(z) \\ &= \psi_{q+1}(z) + (\alpha_{q+1} - \alpha_1)\psi_q(z) - \beta_{q+1}\psi_{q-1}(z) \end{aligned}$$

for  $q = 0, 1, 2, \dots$ , it follows that  $M_t^{(1)}$  is given by

$$M_t^{(1)} = [m_{p,q+1} + (\alpha_{q+1} - \alpha_1)m_{p,q} - \beta_{q+1}m_{p,q-1}]_{p,q=0}^{t-1}.$$

If all the  $\beta_k$ 's are equal to zero, i.e., if

$$\psi_k(z) = (z - \alpha_1)\cdots(z - \alpha_k), \quad k = 1, 2, \dots,$$

then

$$M_t^{(1)} = [m_{p,q+1} + (\alpha_{q+1} - \alpha_1)m_{p,q}]_{p,q=0}^{t-1}.$$

If all the  $\beta_k$ 's are equal to zero and all the  $\alpha_k$ 's are equal to  $\alpha$ , i.e., if

$$\psi_k(z) = (z - \alpha)^k, \quad k = 1, 2, \dots,$$

then

$$m_{p,q} = \frac{1}{2\pi i} \int_{\gamma} (z - \alpha)^{p+q} \frac{f'(z)}{f(z)} dz$$

for  $p, q = 0, 1, 2, \dots$ , and thus  $M_k$  as well as  $M_k^{(1)}$  are Hankel matrices for all  $k$ . If  $\alpha = 0$ , then we are back in the case discussed in the introduction.

By now the reader will probably have realized that we plan to calculate the zeros  $z_1, \dots, z_n$  from the eigenvalues of the pencil  $G_n^{(1)} - \lambda G_n$ . Indeed, as already shown in the introduction, numerical experiments indicate that this approach gives accurate results. This does not come as a complete surprise of course. The system of polynomial equations  $\sum_{k=1}^n \nu_k z_k^p = s_p$ ,  $p = 0, 1, \dots, 2n - 1$ , has the same structure as the system that determines a Gauss quadrature formula, and in numerical integration quadrature formulae are constructed from modified moments based on orthogonal polynomials [6].

To calculate the matrices  $G_n$  and  $G_n^{(1)}$  we need the polynomials  $\varphi_0, \varphi_1, \dots, \varphi_{n-1}$ . The regular FOPs in this sequence can be computed by solving generalized eigenvalue problems, and it is advantageous to define the inner polynomials by using the standard monomial basis, because then the blocks in  $G_k$  and  $G_k^{(1)}$  will have Hankel structure. The following example explains the details of this approach. (Note that we still assume that we are able to calculate all the ‘‘inner products’’  $\langle \cdot, \cdot \rangle$  that are needed exactly, as if we had an ‘‘oracle’’ at our disposal that provides us with the exact value of any inner product upon simple request. In practice, of course, we will have to

calculate inner products via numerical integration. We will have more to say about this in the next section.) We start by calculating—by asking our oracle for—the value of  $s_0$ . Suppose that we find that  $s_0 = 10$ . Then we compute  $s_1$  to obtain the arithmetic mean of the zeros  $\mu = s_1/s_0$ . Now we already know the polynomials  $\varphi_0(z) = 1$  and  $\varphi_1(z) = z - \mu$ , and we proceed by calculating  $\langle \varphi_1, \varphi_1 \rangle$ . Suppose that we find that this inner product is different from zero. This identifies  $\varphi_2$  as a regular FOP. By calculating the eigenvalues  $\lambda_1$  and  $\lambda_2$  of the pencil

$$G_2^{(1)} - \lambda G_2 = \begin{bmatrix} 0 & \langle \varphi_1, \varphi_1 \rangle \\ \langle \varphi_1, \varphi_1 \rangle & \langle \varphi_1, \varphi_1^2 \rangle \end{bmatrix} - \lambda \begin{bmatrix} s_0 & 0 \\ 0 & \langle \varphi_1, \varphi_1 \rangle \end{bmatrix}$$

we obtain  $\varphi_2$  as  $\varphi_2(z) = (z - (\lambda_1 + \mu))(z - (\lambda_2 + \mu))$ . Next we compute  $\langle \varphi_2, \varphi_2 \rangle$ . Suppose that we find that  $\langle \varphi_2, \varphi_2 \rangle = 0$ . This implies that we will have to define  $\varphi_3$  as an inner polynomial. Now there are two possibilities: either  $n = 2$  or  $n > 2$ . In the former case  $\langle z^t \varphi_2, \varphi_2 \rangle = 0$  for every integer  $t \geq 0$ , while in the latter case there exists an integer  $\tau \geq 1$  with  $\tau + 2 \leq n - 1$  such that  $\langle z^t \varphi_2, \varphi_2 \rangle = 0$  for  $t = 0, 1, \dots, \tau - 1$  and  $\langle z^\tau \varphi_2, \varphi_2 \rangle \neq 0$ . The length of the block of polynomials that starts with  $\varphi_2$  will then be equal to  $\tau + 1$ . Thus we proceed by computing  $\langle z \varphi_2, \varphi_2 \rangle, \langle z^2 \varphi_2, \varphi_2 \rangle, \dots$ . Suppose that we find that  $\langle z \varphi_2, \varphi_2 \rangle = 0$  and  $\langle z^2 \varphi_2, \varphi_2 \rangle \neq 0$ . Then we may conclude that  $\varphi_3$  as well as  $\varphi_4$  have to be defined as inner polynomials and that  $\varphi_5$  is a regular FOP. We set  $\varphi_3(z) := z \varphi_2(z)$  and  $\varphi_4(z) := z^2 \varphi_2(z)$ . (In general we have the following. Let  $\varphi_r$  be a regular FOP such that  $\langle \varphi_r, \varphi_r \rangle = 0$ . If  $r = N$  or  $r = N - 1$ , then we may conclude that  $n = r$  and stop. Else we scan the sequence  $\langle z \varphi_r, \varphi_r \rangle, \dots, \langle z^{N-1-r} \varphi_r, \varphi_r \rangle$  for its first nonzero element. If all these inner products are equal to zero, then  $n = r$  and we may stop. Else we know that  $n > r$ , we have determined the length of the block of polynomials that starts with  $\varphi_r$ , and we can proceed to determine the next regular FOP.) Next we obtain  $\varphi_5$  by computing the eigenvalues of the pencil  $G_5^{(1)} - \lambda G_5$ . The matrices  $G_5$  and  $G_5^{(1)}$  are given by

$$G_5 = \begin{bmatrix} s_0 & 0 & 0 & 0 & 0 \\ 0 & \langle \varphi_1, \varphi_1 \rangle & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \langle z^2 \varphi_2, \varphi_2 \rangle \\ 0 & 0 & 0 & \langle z^2 \varphi_2, \varphi_2 \rangle & \langle z^3 \varphi_2, \varphi_2 \rangle \\ 0 & 0 & \langle z^2 \varphi_2, \varphi_2 \rangle & \langle z^3 \varphi_2, \varphi_2 \rangle & \langle z^4 \varphi_2, \varphi_2 \rangle \end{bmatrix}$$

and

$$G_5^{(1)} = \begin{bmatrix} 0 & \langle \varphi_1, \varphi_1 \rangle & 0 & 0 & 0 \\ \langle \varphi_1, \varphi_1 \rangle & \langle \varphi_1, \varphi_1^2 \rangle & 0 & 0 & \langle z^2 \varphi_2, \varphi_2 \rangle \\ 0 & 0 & 0 & \langle z^2 \varphi_2, \varphi_2 \rangle & \langle z^2 \varphi_2, \varphi_1 \varphi_2 \rangle \\ 0 & 0 & \langle z^2 \varphi_2, \varphi_2 \rangle & \langle z^2 \varphi_2, \varphi_1 \varphi_2 \rangle & \langle z^3 \varphi_2, \varphi_1 \varphi_2 \rangle \\ 0 & \langle z^2 \varphi_2, \varphi_2 \rangle & \langle z^2 \varphi_2, \varphi_1 \varphi_2 \rangle & \langle z^3 \varphi_2, \varphi_1 \varphi_2 \rangle & \langle z^4 \varphi_2, \varphi_1 \varphi_2 \rangle \end{bmatrix}.$$

Next we calculate  $\langle \varphi_5, \varphi_5 \rangle$ . Suppose that we find that  $\langle \varphi_5, \varphi_5 \rangle \neq 0$ . Then we may proceed to compute the regular FOP  $\varphi_6$  by calculating the eigenvalues of the pencil  $G_6^{(1)} - \lambda G_6$ . Suppose that we find that  $\langle \varphi_6, \varphi_6 \rangle = 0$  and that  $\langle z^t \varphi_6, \varphi_6 \rangle = 0$  for  $t = 1, \dots, N - 1 - 6$ . This implies that  $n = 6$  and we may stop. We have found that  $f$  has six mutually distinct zeros in the interior of  $\gamma$ . They are given by the zeros of  $\varphi_6$  (which we obtained from the eigenvalues of  $G_6^{(1)} - \lambda G_6$ ). Their corresponding multiplicities are found by solving the Vandermonde-like system (6).

In practice, however, life will not be all that easy. 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. However, from a numerical point of view a test “is equal to zero” does not make sense. By evaluating the corresponding integrals numerically, we will obtain accurate approximations for the inner products but not their exact values. If we would apply the algorithm that we have just described “as is,” we would encounter only regular FOPs. Strictly speaking we 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 [5, 2, 1]. In this approach the blocks  $\langle \Phi, \Phi \rangle$  in  $G$  are taken (slightly) larger than strictly necessary to avoid ill-conditioned blocks. A disadvantage is that part of the structure of  $G$  and  $G^{(1)}$  gets lost. Suppose  $\Phi := [\varphi_r \quad z\varphi_r \quad \cdots \quad z^{l-1}\varphi_r]$  is a block of length  $l$  that starts with a (well-conditioned) regular FOP. The matrix  $\langle \Phi, \Phi \rangle$  will still be a Hankel matrix of course, but no longer lower triangular. Also there will be some additional fill-in in  $G$  and  $G^{(1)}$  as  $\langle z^\alpha \varphi_r, \varphi_q \rangle$  where  $\alpha \in \{0, 1, \dots, l-1\}$  will be equal to zero only for  $q = 0, 1, \dots, r - \alpha - 1$  and  $\langle z^\alpha \varphi_r, \varphi_1 \varphi_q \rangle = 0$  only for  $q = 0, 1, \dots, r - \alpha - 2$ . We will ask the user for two thresholds,  $\epsilon_{\text{stop}}$  and  $\epsilon_{\text{cond}}$  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  $\varphi_r$ . 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  $\varphi_{r+1}$  as a regular FOP. 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  $t = 0, 1, \dots, N-1-r$  then we conclude that  $n = r$  and stop. Else we search for the first element that is larger than  $\epsilon_{\text{cond}}$ . The corresponding value of  $t$  then determines the size of the block of polynomials. If all the elements are less than  $\epsilon_{\text{cond}}$  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.

**Algorithm.**

**input**  $\langle \cdot, \cdot \rangle, \epsilon_{\text{stop}}, \epsilon_{\text{cond}}$

**output**  $n, \text{zeros}$

**comment**  $\text{zeros} = \{z_1, \dots, z_n\}$ . We assume that  $\epsilon_{\text{stop}} < \epsilon_{\text{cond}}$ .

$N \leftarrow \langle 1, 1 \rangle$

**if**  $N == 0$  **then**

$n \leftarrow 0$ ;  $\text{zeros} \leftarrow \emptyset$ ; **stop**

**else**

$\varphi_0(z) \leftarrow 1$

$\mu \leftarrow \langle z, 1 \rangle / N$ ;  $\varphi_1(z) \leftarrow z - \mu$

$r \leftarrow 1$

**while**  $r < N$  **do**

**if**  $|\langle \varphi_r(z), \varphi_r(z) \rangle| \geq \epsilon_{\text{cond}}$  **then**

generate  $\varphi_{r+1}(z)$  as a regular FOP

$r \leftarrow r + 1$

**else**

$\text{allsmall} \leftarrow \text{true}$ ;  $\text{notfound} \leftarrow \text{true}$ ;  $\text{maximum} \leftarrow 0$ ;  $t \leftarrow 0$

**while**  $\text{notfound}$  **and**  $(t \leq N - 1 - r)$

$\text{ip} \leftarrow |\langle z^t \varphi_r(z), \varphi_r(z) \rangle|$

$\text{allsmall} \leftarrow \text{allsmall}$  **and**  $(\text{ip} < \epsilon_{\text{stop}})$

**comment** search for the smallest  $t \in \{0, 1, \dots, N - 1 - r\}$  such

that  $|\langle z^t \varphi_r(z), \varphi_r(z) \rangle| \geq \epsilon_{\text{cond}}$

**if**  $(\text{ip} \geq \epsilon_{\text{cond}})$  **then**

$\text{notfound} \leftarrow \text{false}$ ;  $\text{tlarge} \leftarrow t$

**end if**

**comment** search for  $\text{tmax} \in \{0, 1, \dots, N - 1 - r\}$  such

that  $|\langle z^{\text{tmax}} \varphi_r(z), \varphi_r(z) \rangle| = \max(|\langle z^t \varphi_r(z), \varphi_r(z) \rangle|)_{t=0}^{N-1-r}$

**if**  $(\text{ip} > \text{maximum})$  **then**

$\text{maximum} \leftarrow \text{ip}$ ;  $\text{tmax} \leftarrow t$

**end if**

$t \leftarrow t + 1$

**end while**

**if**  $\text{notfound}$  **then**

**if**  $\text{allsmall}$  **then**

$n \leftarrow r$ ;  $\text{zeros} \leftarrow \text{roots}(\varphi_r)$ ; **stop**

**else**

```

print "Warning: requested level of well-conditioning is impossible to obtain"
if tmax == 0 then
  print "Warning: you may want to raise the value of  $\epsilon_{\text{stop}}$ "
   $n \leftarrow r$ ; zeros  $\leftarrow$  roots( $\varphi_r$ ); stop
else
  tblock  $\leftarrow$  tmax
end if
end if
else
  tblock  $\leftarrow$  tlarge
end if
for  $\alpha = 1 : \text{tblock}$ 
   $\varphi_{r+\alpha}(z) \leftarrow z^\alpha \varphi_r(z)$ 
end for
  generate  $\varphi_{r+\text{tblock}+1}$  as a regular FOP
   $r \leftarrow r + \text{tblock} + 1$ 
end if
end while
 $n \leftarrow N$ ; zeros  $\leftarrow$  roots( $\varphi_N$ ); stop
end if

```

*Note.* As we represent our formal orthogonal polynomials by using the product representation,  $\varphi(z) = \prod_{\alpha \in \varphi^{-1}(0)} (z - \alpha)$ , the function roots( $\cdot$ ) is obviously *not* a function that calculates the zeros of a polynomial from its coefficients in the standard monomial basis.

#### 4. NUMERICAL EXAMPLES

We have implemented our algorithm in Matlab. The m-files are available from the first author. We will present six numerical examples. In the first three examples we started from the zeros and their respective multiplicities and recalculated them via our algorithm. The inner products were computed explicitly as  $\langle \phi, \psi \rangle = \sum_{k=1}^n \nu_k \phi(z_k) \psi(z_k)$ . In the last three examples we started from an analytic function and calculated the inner products via numerical integration. The computations have been done using Matlab 4.2c (with floating point relative accuracy  $\approx 2.2204 \cdot 10^{-16}$ ).

**Example 1.** Suppose that  $n = 10$ ,

$$z_1 = 1, \quad z_2 = 2, \quad z_3 = 3, \quad z_4 = 4, \quad z_5 = 5, \\ z_6 = 6, \quad z_7 = 7, \quad z_8 = 8, \quad z_9 = 9, \quad z_{10} = 10$$

and  $\nu_1 = \dots = \nu_{10} = 1$ . By calculating the eigenvalues of the pencil  $H_n^< - \lambda H_n$  (as we would have done in [11]) we obtain the approximations

$$0.99997610636668, \quad 1.99812692712904, \quad 2.96964756470803, \\ 3.85164221027260, \quad 4.76929486601830, \quad 5.83891586633208, \\ 6.93895160469148, \quad 7.98903115901926, \quad 8.99931401487053, \quad 9.99999170411583.$$

(The imaginary parts are not shown—they are  $\mathcal{O}(10^{-9})$ .) Our algorithm (with  $\epsilon_{\text{stop}} = 10^{-12}$  and  $\epsilon_{\text{cond}} = 1$ ) generates only regular FOPs, concludes that  $n = 10$  and obtains the (very accurate!) approximations

$$1.00000000000001, \quad 2.00000000000000, \quad 3.00000000000000, \\ 4.00000000000000, \quad 4.99999999999996, \quad 5.99999999999998, \\ 7.00000000000001, \quad 8.00000000000000, \quad 9.00000000000000, \quad 9.99999999999999.$$

(The imaginary parts are  $\mathcal{O}(10^{-15})$ .)

**Example 2.** Zero configurations that necessitate the use of inner polynomials for theoretical reasons (as opposed to reasons of numerical stability) are not difficult to find. Suppose  $n = 3$ ,

$$z_1 = 0, \quad z_2 = \sqrt{3} + i, \quad z_3 = \sqrt{3} - i$$

and  $\nu_1 = \nu_2 = \nu_3 = 1$ . Then  $H_2$  (and thus, by Theorem 7, also  $G_2$ ) is singular. This implies that the regular FOP of degree two does not exist, and indeed our algorithm (with  $\epsilon_{\text{stop}} = 10^{-12}$  and  $\epsilon_{\text{cond}} = 1$ ) decides to define  $\varphi_2$  as an inner polynomial and obtains the (exact!) approximations

$$0.00000000000000, \quad 1.73205080756888 \pm i 1.00000000000000.$$

The choice of  $\epsilon_{\text{stop}}$  and (especially)  $\epsilon_{\text{cond}}$  is of course a difficult one. The next example illustrates what happens if we choose  $\epsilon_{\text{cond}}$  too large.

**Example 3.** Suppose that  $n = 5$ ,

$$z_1 = 1, \quad z_2 = 2, \quad z_3 = 3, \quad z_4 = 4, \quad z_5 = 5$$

and

$$\nu_1 = 2, \quad \nu_2 = 3, \quad \nu_3 = 2, \quad \nu_4 = 3, \quad \nu_5 = 1.$$

Then  $N = 11$ . Our algorithm with  $\epsilon_{\text{stop}} = 10^{-12}$  and  $\epsilon_{\text{cond}} = 1$  generates only regular FOPs, decides correctly that  $n = 5$  and obtains the approximations

$$1.00000000000000, \quad 2.00000000000000, \\ 3.00000000000000, \quad 4.00000000000001, \quad 5.00000000000000$$

and the correct corresponding multiplicities. However, if we put  $\epsilon_{\text{cond}} = 100$  then our algorithm concludes that  $n = 7$  and it generates only  $\varphi_0, \varphi_1, \varphi_4$  and  $\varphi_7$  as regular FOPs. The approximations for the zeros and the rounded values of the computed multiplicities are shown in the following table.

$0.99999999999909 + i 0.00000000000040$	2
$2.00000000000007 - i 0.00000000000002$	3
$2.99999999999997 + i 0.00000000000001$	2
$4.00000000000000 + i 0.00000000000002$	3
$4.99999999999999 + i 0.00000000000002$	1
$0.48975270960595 + i 0.16173423694917$	0
$1.36957420453839 + i 0.13575736551242$	0

The spurious zeros (cf. Theorem 3 and its generalization Theorem 8) can easily be removed by inspecting the computed multiplicities. Note that the approximations for the actual zeros are still quite accurate.

If  $\gamma$  is a circle with centre  $c$  and radius  $\rho$ , then

$$(7) \quad \langle \phi, \psi \rangle = \rho \int_0^1 \phi(c + \rho e^{2\pi i \theta}) \psi(c + \rho e^{2\pi i \theta}) \frac{f'(c + \rho e^{2\pi i \theta})}{f(c + \rho e^{2\pi i \theta})} e^{2\pi i \theta} d\theta.$$

Since this is the integral of a periodic function over a complete period, the trapezoidal rule is an appropriate quadrature rule. If  $F : [0, 1] \rightarrow \mathbb{C}$  is the integrand in the right hand side of (7), then the  $q$ -point trapezoidal rule approximation to  $\langle \phi, \psi \rangle$  is given by

$$\langle \phi, \psi \rangle = \int_0^1 F(\theta) d\theta \approx \frac{1}{q} \sum_{k=0}^{q-1} F(k/q) =: T_q.$$

The double prime indicates that the first and the last term of the sum are to be multiplied by  $1/2$ . As  $F$  is periodic with period one, we may rewrite  $T_q$  as

$$T_q = \frac{1}{q} \sum_{k=0}^{q-1} F(k/q).$$

This shows that  $T_q$  indeed depends on  $q$  (and not  $q + 1$ ) points. As

$$T_{2q} = \frac{1}{2}T_q + \frac{1}{2q} \sum_{k=0}^{q-1} F\left(\frac{2k+1}{2q}\right),$$

successive doubling of  $q$  enables us in each step to reuse the integrand values needed in the previous step. In the following examples we started with  $q = 1$  and continued doubling  $q$  until  $|T_{2q} - T_q|$  was sufficiently small.

Lyness and Delves [13] have studied the asymptotic behaviour of the quadrature error. They have shown that the modulus of the error made by the  $q$ -point trapezoidal rule is asymptotically  $\mathcal{O}(A^q)$  where  $0 \leq A < 1$ . More precisely,

$$A := \max\left\{\frac{|z_I|}{\rho}, \frac{\rho}{|z_E|}, \frac{\rho}{\rho_s}\right\}$$

where  $z_I$  is the zero of  $f$  that lies closest to  $\gamma$  and in the interior of  $\gamma$ ,  $z_E$  is the zero of  $f$  that lies closest to  $\gamma$  and in the exterior of  $\gamma$ , and  $\rho_s$  is the distance between  $c$  and the nearest singularity of  $f$ .

To assess the accuracy of our algorithm, in the following examples the approximations for the zeros have been refined iteratively via Newton's method

$$z_k^{(\alpha+1)} = z_k^{(\alpha)} - \nu_k \frac{f(z_k^{(\alpha)})}{f'(z_k^{(\alpha)})}, \quad \alpha = 0, 1, 2, \dots$$

The underlined digits in the approximations obtained by our algorithm were correct.

**Example 4.** Let  $f(z) := e^{3z} + 2z \cos z - 1$  and  $\gamma := \{z \in \mathbb{C} : |z| = 2\}$ . Our algorithm with  $\epsilon_{\text{stop}} = 10^{-12}$  and  $\epsilon_{\text{cond}} = 1$  finds that  $N = 4$ . It generates  $\varphi_1$  as a regular FOP, defines  $\varphi_2$  as an inner polynomial, generates  $\varphi_3$  and  $\varphi_4$  as regular FOPs and concludes that  $n = 4$ . The approximations for the zeros and the corresponding multiplicities are shown in the following table.

<u>-1.84423395326221</u> + $i$ <u>0.00000000000000</u>	1
<u>0.53089493029293</u> + $i$ <u>1.33179187675112</u>	1
<u>0.53089493029293</u> - $i$ <u>1.33179187675112</u>	1
<u>0.00000000000000</u> + $i$ <u>0.00000000000000</u>	1

The calculated multiplicities were at a distance of  $\mathcal{O}(10^{-15})$  to integers.

If we put  $\epsilon_{\text{cond}} = 0.1$  then our algorithm generates only regular FOPs. Now the approximations for the zeros are less accurate.

<u>-1.84423395326194</u> - $i$ <u>0.00000000000499</u>	1
<u>0.53089493028783</u> + $i$ <u>1.33179187675442</u>	1
<u>0.53089493029794</u> - $i$ <u>1.33179187674729</u>	1
<u>-0.00000000000071</u> - $i$ <u>0.00000000000211</u>	1

This illustrates the importance of generating only well-conditioned regular FOPs. The calculated multiplicities were at a distance of  $\mathcal{O}(10^{-11})$  to integers.

**Example 5.** Let  $f(z) := z^2(z-1)(z-2)(z-3)(z-4) + z \sin z$  and  $\gamma := \{z \in \mathbb{C} : |z| = 5\}$ . Our algorithm with  $\epsilon_{\text{stop}} = 10^{-12}$  and  $\epsilon_{\text{cond}} = 1$  finds that  $N = 6$ . It generates  $\varphi_1, \varphi_2, \varphi_3, \varphi_4$  and  $\varphi_5$  as regular FOPs. Then it warns us that the requested level of well-conditioning is impossible to obtain, it tells us that we may want to raise the value of  $\epsilon_{\text{stop}}$  and concludes (correctly) that  $n = 5$ . The approximations for the zeros and the corresponding multiplicities are shown in the following table.

<u>0.00000000000018</u> + $i$ <u>0.00000000000069</u>	2
<u>1.18906588973121</u> + $i$ <u>0.000000000008087</u>	1
<u>1.72843498615571</u> + $i$ <u>0.00000000012431</u>	1
<u>3.01990732809215</u> + $i$ <u>0.00000000002162</u>	1
<u>4.03038191606022</u> + $i$ <u>0.00000000000173</u>	1

The computed multiplicities were at a distance of  $\mathcal{O}(10^{-12})$  to integers. Let us try to explain what caused the warnings. Our function  $f$  has a double zero at the origin. Thus  $n = 5$  and theoretically  $\langle \varphi_5, \varphi_5 \rangle = 0$ . However, as by evaluating the inner products via numerical integration we can only obtain approximations for them, the original well-conditioned problem consisting of four simple zeros and one double zero is perturbed into an ill-conditioned problem where the double zero is split into two simple zeros that lie close to each other. This explains why  $\epsilon_{\text{stop}} < |\langle \varphi_5, \varphi_5 \rangle| < \epsilon_{\text{cond}}$ . By raising the value of  $\epsilon_{\text{stop}}$  we coalesce these two simple zeros into one double zero.

Our last example is a mixture of Examples 3 and 5.

**Example 6.** Let  $f(z) := z^2(z-2)^2[\cos ze^{2z} + z^3 - 1 - \sin z]$  and  $\gamma := \{z \in \mathbb{C} : |z| = 3\}$ . Our algorithm with  $\epsilon_{\text{stop}} = 10^{-12}$  and  $\epsilon_{\text{cond}} = 1$  finds that  $N = 8$ . It generates  $\varphi_1, \varphi_2, \varphi_3, \varphi_4$  and  $\varphi_5$  as regular FOPs, then warns us that the requested level of well-conditioning is impossible to obtain, defines  $\varphi_6$  and  $\varphi_7$  as inner polynomials, generates  $\varphi_8$  as a regular FOP and stops. The approximations for the zeros and the corresponding multiplicities are shown in the following table.

$0.00000000000351 + i 0.00000000000910$	3
$1.99999999999999 - i 0.00000000000001$	2
$1.66468286974521 - i 0.00000000000011$	1
$-0.46071411972767 + i 0.62542776934861$	1
$-0.46071411972707 - i 0.62542776934724$	1
$1.72060314137159 + i 1.85484636500232$	0
$0.14700911592711 - i 0.22187905247210$	0
$-2.95622283859992 - i 1.93675565998980$	0

It follows that  $n$  is actually equal to five and that the last three “zeros” are spurious. The calculated multiplicities were at a distance of  $\mathcal{O}(10^{-11})$  to integers.

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