ELSEVIER Linear Algebra and its Applications 280 (1998) 129–162

LINEAR ALGEBRA AND ITS APPLICATIONS

Krylov subspace methods for eigenvalues with special properties and their analysis for normal matrices [1]

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Received 30 January 1996; received in revised form 31 October 1997; accepted 28 January 1998

Submitted by M. Goldberg

Abstract

In this paper we propose a general approach by which eigenvalues with a special property of a given matrix A can be obtained. In this approach we first determine a scalar function $\psi : \mathbb{C} \to \mathbb{C}$ whose modulus is maximized by the eigenvalues that have the special property. Next, we compute the generalized power iterations $u_{j+1} = \psi(A)u_j$, $j = 0, 1, \ldots$, where u_0 is an arbitrary initial vector. Finally, we apply known Krylov subspace methods, such as the Arnoldi and Lanczos methods, to the vector u_n for some sufficiently large n. We can also apply the simultaneous iteration method to the subspace $\text{span}\{x_1^{(n)}, \ldots, x_k^{(n)}\}$ with some sufficiently large n, where $x_m^{(j+1)} = \psi(A)x_m^{(j)}$, $j = 0, 1, \ldots$, $m = 1, \ldots, k$. In all cases the resulting Ritz pairs are approximations to the eigenpairs of A with the special property. We provide a rather thorough convergence analysis of the approach involving all three methods as $n \to \infty$ for the case in which A is a normal matrix. We also discuss the connections and similarities of our approach with the existing methods and approaches in the literature.

Keywords: Eigenvalue problems; Special eigenvalues; Power iterations; Krylov subspace methods; Normal matrices

[1] The results of this paper were presented at the AMS-SIAM Summer Seminar: Mathematics of Numerical Analysis, Park City, Utah, July–August 1995.

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0024-3795/98/$19.00
PII: S0024-3795(98)10029-0

1. Introduction

Let A be an $N \times N$ matrix that is in general complex and denote its eigenvalues by μ_i, $i = 1, 2, \ldots, N$. In some applications we may need to find a number of the eigenvalues of A that have some special property and their corresponding invariant subspaces. For example, we may need some of those μ_i:

(i) that have largest moduli, or

(ii) that have largest real parts, or

(iii) that lie in a given set Ω in the complex plane, etc.

We assume that corresponding to the special property considered there exists a scalar function $\psi(\mu), \psi : \mathbb{C} \to \mathbb{C}$ such that the eigenvalues satisfying this special property maximize $|\psi(\mu)|$. If we order the eigenvalues μ_i of A such that

$$|\psi(\mu_1)| \geqslant |\psi(\mu_2)| \geqslant |\psi(\mu_3)| \geqslant \cdots, \tag{1.1}$$

then we are interested in finding $\mu_1, \mu_2, \ldots$, in this order. Hence, our task can be reformulated to read as follows: Given the function $\psi : \mathbb{C} \to \mathbb{C}$ and the ordering of the μ_i in Eq. (1.1), find $\mu_1, \mu_2, \ldots, \mu_k$ for a given integer k.

Going back to the above examples, we see that the most obvious candidates for $\psi(\mu)$ are as follows:

(i) For eigenvalues that are largest in modulus, $\psi(\mu) = \mu$.

For eigenvalues with largest real parts, $\psi(\mu) = \exp(\mu)$.

(iii) For eigenvalues in a set Ω of the complex plane, pick $\psi(\mu)$ to be, for example, a polynomial, whose modulus assumes its largest values on Ω and is relatively small on the rest of the spectrum of A. (The behavior of $\psi(\mu)$ outside the spectrum of A is immaterial.)

As we shall see in Section 2, the function $\psi(\mu)$ enters the picture through the computation of the *vectors* $\psi(A)u \in \mathbb{C}^N$, where $\psi(A)$ is an $N \times N$ matrix and $u \in \mathbb{C}^N$. The computation of the *matrix* $\psi(A)$, which may be a prohibitively expensive task even in the simplest cases, is *not* necessary for this purpose. The *vectors* $\psi(A)u$ can be computed exactly in case $\psi(\mu)$ is a polynomial or can be approximated by $\hat{\psi}(A)u$, where $\hat{\psi}(\mu)$ is an appropriate polynomial approximation for $\psi(\mu)$.

The purpose of the present work is to consider a general approach that has been observed to achieve the task above in some special cases. An important ingredient of this approach is the use of any one of the following three methods that are employed in approximating a number of eigenvalues of a given matrix: (1) The method of Arnoldi [1], (2) the method of Lanczos [12], and (3) the simultaneous iteration method (see the references in [7], Sections 7.3 and 8.5). Thus, this general approach is really a collection of three different methods which we call the Special Eigenvalue Arnoldi, Lanczos, and Simultaneous Iteration methods. We will denote these methods by SEA, SEL, and SESI, respectively, for short. (Of course, we can employ additional methods for the partial

solution of the eigenvalue problem, such as the block Arnoldi and block Lanczos methods, thus enlarging this collection.) After describing how these methods can be applied to find eigenvalues with special properties, we provide a detailed analysis of convergence for the case in which the matrix A is normal. (We propose to extend this analysis to the case of nonnormal matrices in a future publication although we mention the relevant results in appropriate places of this work.)

The plan of the present work is as follows: In Section 2 we treat the simplest problem of finding μ_1 and a corresponding eigenvector. The method that we propose and analyze there is an extension of the power method (it is actually the power method when $\psi(\mu) = \mu$). This may serve as a motivation for the general approach and contains some of the major ingredients of this approach.

In Section 3 we describe briefly the Arnoldi and Lanczos methods and the simultaneous iteration method. Our description is mathematical; we do not dwell on the important issue of numerical implementations of these methods. Following this, in Section 4 we describe fully the approach to the solution of the special eigenvalue problem using SEA, SEL, and SESI.

The convergence analysis of this general approach for the case in which A is normal is the subject of Sections 5–8. In Section 5 we provide some theoretical preliminaries that are crucial for a proper understanding of the results of Sections 6–8 and their proofs. The main results of these sections are Theorem 6.3 on convergence to eigenvalues, Theorem 7.1 on convergence to eigenvectors, and Theorem 8.1 on formation of spurious eigenvalues under some conditions. An interesting feature of our treatment is that it allows us to give a *unified* analysis of all three methods that we employ. The mathematics that is used in this analysis has been placed in Appendix A. We believe that some of the results in Appendix A are of independent interest.

In Section 9 we provide numerical examples by which we demonstrate some of the theoretical results of Sections 6 and 7.

The problem of finding eigenvalues with special properties has received some attention in the past. First, it is well known that when applied to a hermitian matrix the (symmetric) Lanczos method produces approximations to the largest and the smallest eigenvalues whose accuracy increases with the size of the underlying Krylov subspace. The same holds true for the block Lanczos method, see [4,6]. This has been analyzed in [11,13,17] for the Lanczos method, and in [28] for the block Lanczos method (see also [14,7]). Next, the use of Chebyshev polynomials for improving the convergence of the subspace iteration method for hermitian matrices was proposed in [15,16]. The approach in these two papers was generalized in [19] to improve the convergence of the Arnoldi method and the subspace iteration method for eigenvalues with largest real parts of nonhermitian matrices. We will comment on these in Section 4.

We now mention those methods that are exactly of the form that we treat in this work and that have been suggested and applied in the past.

The simultaneous iteration method was designed to find a number of eigenvalues with largest moduli with $\psi(\mu) = \mu$ for this method. The literature for it is quite extensive. See, for example [8,2,3,25,26,15,16,29,10,27]. See also the books [9,14,7]. A convergence analysis for hermitian matrices is given in [25], while [26] provides an analysis for nonhermitian matrices. The use of the Arnoldi and Lanczos methods for finding a number of eigenvalues with largest moduli was proposed in [23] with $\psi(\mu) = \mu$ in this case too. The treatment of [23] includes general nondiagonalizable matrices and normal matrices as well. It provides the constructions of eigenvalue and invariant subspace approximations, and contains a complete convergence theory for all cases. This theory is based on the connection of the Arnoldi and Lanczos methods with certain vector-valued rational approximations that have been studied in [22]. The treatment of eigenvalues with largest moduli of normal matrices by the Arnoldi method was previously given in [20] again with $\psi(\mu) = \mu$.

The problem of finding eigenvalues with largest real parts was tackled in [5] with $\psi(\mu) = \exp(\mu)$ explicitly. The vectors $u_n = [\psi(A)]^n u_0 = e^{nA} u_0$ that are needed are approximated through the numerical solution of the linear system of ordinary differential equations $u'(t) = Au(t)$ with initial conditions $u(0) = u_0$, where $u(n) \equiv u_n$. Subsequently, a mathematical equivalent of the Arnoldi method is employed. (This equivalence can be verified with the help of [23], Section 5.) The method then is applied to a problem in hydrodynamic stability that involves the Orr–Sommerfeld equation.

Finally, the techniques of analysis in the present work form an extension of those developed in [20]. These techniques are nongeometric in the sense that they do not utilize projection operators.

2. A power method for μ_1

To motivate our approach we will start with the problem of finding only that eigenvalue of A that maximizes $|\psi(\mu)|$, namely, μ_1 in Eq. (1.1), and a corresponding eigenvector. For simplicity we assume that A is diagonalizable. The method that we propose below is a generalization of the power method via the Rayleigh quotient. It is also a special case of SEA as will be explained later.

We start by picking an arbitrary vector $u_0 \in \mathbb{C}^N$. We next generate the vectors $u_1, u_2, \ldots$, through $u_{j+1} = \psi(A)u_j$, $j = 0, 1, 2, \ldots$ (Obviously, in computational work we would normalize these vectors as we generate them.) We then compute the Rayleigh quotient

$$\rho_n = \frac{(u_n, Au_n)}{(u_n, u_n)} \tag{2.1}$$

with $(a, b) = a^* Q b$, where Q is some hermitian positive definite matrix. Theorem 2.1 below states the precise conditions under which ρ_n tends to μ_1 and a

properly normalized u_n tends to an eigenvector corresponding to μ_1. We leave the proof of this theorem to the reader.

Theorem 2.1. *Denote the eigenvector of A that corresponds to the eigenvalue μ_i by v_i, $i = 1, 2, \ldots, N$. For some $r \geq 1$ we have $\mu_1 = \mu_2 = \cdots = \mu_r \neq \mu_{r+1}$. Also, $u_0 = \sum_{i=1}^{N} \gamma_i v_i$ for some scalars γ_i. Assume that $\psi(A)v_i = \psi(\mu_i)v_i$ for all i. Provided that*

$$|\psi(\mu_r)| > |\psi(\mu_{r+1})| \quad \text{and} \quad \sum_{i=1}^{r} |\gamma_i| \neq 0, \tag{2.2}$$

we have

$$\rho_n - \mu_1 = \mathrm{O}\left(\left| \frac{\psi(\mu_{r+1})}{\psi(\mu_r)} \right|^n \right) \quad \text{as } n \to \infty, \tag{2.3}$$

and, for some normalization constant α_n,

$$\alpha_n u_n - \sum_{i=1}^{r} \gamma_i v_i = \mathrm{O}\left(\left| \frac{\psi(\mu_{r+1})}{\psi(\mu_r)} \right|^n \right) \quad \text{as } n \to \infty. \tag{2.4}$$

If the matrix A is normal, i.e., $A^*A = AA^*$, and $(y, z) = y^*z$, then Eq. (2.3) is improved to read

$$\rho_n - \mu_1 = \mathrm{O}\left(\left| \frac{\psi(\mu_{r+1})}{\psi(\mu_r)} \right|^{2n} \right) \quad \text{as } n \to \infty, \tag{2.5}$$

while Eq. (2.4) remains unchanged.

Note that as $\mu_1 = \cdots = \mu_r$, the vector $\sum_{i=1}^{r} \gamma_i v_i$ is an eigenvector of A corresponding to μ_1. It is also nonzero since $\sum_{i=1}^{r} |\gamma_i| \neq 0$ and $v_1, \ldots, v_r$ are linearly independent.

Obviously, Theorem 2.1 does *not* cover, for instance, the case in which $\mu_2 = \overline{\mu_1}$ and ψ is a real function, for in this case $|\psi(\mu_1)| = |\psi(\mu_2)|$, contrary to Eq. (2.2). This case *is* covered, however, by the theorems of Sections 6 and 7 (with $k \geq 2$ there).

Note 2.1. It is important to emphasize that the method analyzed in Theorem 2.1 is not the standard power method for the matrix $B \equiv \psi(A)$ (for which $\rho_n = (u_n, Bu_n)/(u_n, u_n)$ with $u_n = B^n u_0 = [\psi(A)]^n u_0, n = 1, 2, \ldots$) just as it is not the standard power method for the matrix A (for which $\rho_n = (u_n, Au_n)/(u_n, u_n)$ with $u_n = A^n u_0$, $n = 1, 2, \ldots$). It is the Rayleigh quotient method for the matrix A, the relevant power iterations being $\{[\psi(A)]^m u_0\}$ and not $\{A^m u_0\}$. As such, it seems to be new.

Before we go on we would like to mention that the generation of the vectors $u_1, u_2, \ldots,$ through $u_{j+1} = \psi(A)u_j$, $j = 0, 1, \ldots,$ in the power method above,

forms the first part of SEA and SEL. The importance of this step stems from the fact that the vectors $u_n = [\psi(A)]^n u_0$ have spectral decompositions with large contributions from the invariant subspace of A associated with μ_1. Also, this power method is a special case (the simplest case) of SEA and SESI as will become clear later.

3. A brief description of projection methods for eigenvalue problems

An effective way of obtaining approximations to some of the eigenvalues of a matrix A is through projection methods. In these methods one picks two k-dimensional subspaces Y and Z,

$$Y = \text{span}\{y_1, y_2, \ldots, y_k\} \quad \text{and} \quad Z = \text{span}\{z_1, z_2, \ldots, z_k\}. \tag{3.1}$$

Then an approximate eigenpair (μ, z) is defined by the requirements

$$z \in Z \quad \text{and} \quad (y, Az - \mu z) = 0 \ \text{ for all } y \in Y, \tag{3.2}$$

where $(a, b) \equiv a^* Q b$ for some hermitian positive definite matrix Q. If we also define the matrices Y and Z by

$$Y = [y_1 | y_2 | \cdots | y_k] \quad \text{and} \quad Z = [z_1 | z_2 | \cdots | z_k], \tag{3.3}$$

then, by the fact that $z \in Z$ implies $z = Z\xi$ for some $\xi \in \mathbb{C}^k$, the second requirement in Eq. (3.2) can be expressed equivalently as

$$Y^* Q (A - \mu I) Z \xi = 0. \tag{3.4}$$

Thus μ is an eigenvalue of the $k \times k$ matrix pencil (Y^*QAZ, Y^*QZ) and ξ is the corresponding eigenvector. In the literature μ is called a Ritz value and $z = Z\xi$ is called the corresponding Ritz vector. In general, there will be k pairs of Ritz values and Ritz vectors. Also, the subspaces Y and Z are called the left and right subspaces, respectively. Note that a projection method is uniquely defined by its left and right subspaces Y and Z and by the inner product (or, equivalently, by the matrix Q).

The Arnoldi and Lanczos methods and the simultaneous iteration method are all projection methods with their left and right subspaces as described below. For their efficient implementation we refer the reader to the literature cited in Section 1. A summary of the implementations of the Arnoldi and Lanczos methods can also be found in [23].

For the Arnoldi method

$$Z = \text{span}\{u, Au, \ldots, A^{k-1}u\} \quad \text{and} \quad Y = Z, \tag{3.5}$$

where u is some given vector. For some error bounds, see [18]. If we pick $u = A^n u_0$ for some u_0, then this method produces Ritz values and Ritz vectors that converge, respectively, to eigenvalues of largest modulus and to their

invariant subspaces, as $n \to \infty$. For this theory and some optimality properties of the Arnoldi method, see [23].

For the Lanczos method

$$Z = \text{span}\{u, Au, \ldots, A^{k-1}u\} \quad \text{and} \quad Y = \text{span}\{q, A^*q, \ldots, A^{*k-1}q\}, \tag{3.6}$$

where u and q are some given vectors. For different convergence theories pertaining to hermitian matrices, see [11,13,17]. If we pick $u = A^n u_0$ for some u_0, then this method too produces Ritz values and Ritz vectors that converge, respectively, to eigenvalues of largest modulus and to their invariant subspaces, as $n \to \infty$. For this theory, see [23].

The simultaneous iteration method was designed to produce Ritz values that approximate the eigenvalues of A that are largest in modulus. In this method one begins with a k-dimensional subspace that is spanned by a given set of vectors $w_1, \ldots, w_k$. Then one proceeds through a number of stages at each of which this subspace is modified. It can be shown that at the nth stage this method is a projection method with right and left subspaces given by

$$Z = \text{span}\{w_1^{(n)}, w_2^{(n)}, \ldots, w_k^{(n)}\} \quad \text{and} \quad Y = Z, \tag{3.7}$$

where $w_i^{(n)} = A^n w_i$, $i = 1, \ldots, k$. Again convergence takes place as $n \to \infty$, see [25,26]. See also [15].

In connection with the Lanczos method, we note that when A is hermitian, i.e., $A^* = A$, then with the choice $q = u$ in Eq. (3.6) this method becomes mathematically equivalent to that of Arnoldi.

It is clear that setting up the subspace Z in the simultaneous iteration method is about k times as expensive as setting up Z in the Arnoldi method, when measured in terms of matrix–vector products.

4. Algorithms for eigenvalues with special properties

We now turn to the description of the methods SEA, SEL, SESI by which we would like to approximate the eigenvalues of A that have the special property quantified via the function $\psi(\mu)$.

For SEA we start by picking $u_0 \in \mathbb{C}^N$ arbitrarily, and generate the vectors $u_1, u_2, \ldots,$ by $u_{j+1} = \psi(A)u_j$, $j = 0, 1, \ldots$ We next apply the Arnoldi method with the subspaces Y and Z as in Eq. (3.5), where $u = u_n$ for some large n.

For SEL we start by picking $u_0 \in \mathbb{C}^N$ arbitrarily, and generate the vectors $u_1, u_2, \ldots,$ by $u_{j+1} = \psi(A)u_j$, $j = 0, 1, \ldots$ We next apply the Lanczos method with the subspaces Y and Z as in Eq. (3.6), where $q = u = u_n$ for some large n.

For SESI we start by picking $x_1^{(0)}, \ldots, x_k^{(0)} \in \mathbb{C}^N$ arbitrarily. (These vectors must be linearly independent.) Following that we generate the vectors $x_i^{(1)}, x_i^{(2)}, \ldots,$ by $x_i^{(j+1)} = \psi(A)x_i^{(j)}$, $j = 0, 1, \ldots,$ $i = 1, \ldots, k$. We next apply one

stage of the simultaneous iteration method with the subspaces Y and Z as in Eq. (3.7), where $w_i^{(n)} = x_i^{(n)}$, $i = 1, 2, \ldots, k$, for some large n.

Note that in computational work the vectors u_j and $x_i^{(j)}$, $i = 1, \ldots, k$, should be normalized as they are generated. Obviously, this has no effect whatsoever on the Ritz values and Ritz vectors. Note also that, with $k = 1$, SEA and SESI reduce to the generalized power method treated in Theorem 2.1.

Note 4.1. We emphasize here that the Krylov subspace methods above are being applied with the matrix A and *not* with the matrix $\psi(A)$, and that the corresponding Ritz values will be shown to approximate $\mu_1, \mu_2, \ldots$, directly. This will be done in Section 6.

Before we go on we would like to remark that the use of Chebyshev polynomials in [15,16,19] that we mentioned in Section 1 resembles the approach that we have described above. In [15,16] the subspace Z in the simultaneous iteration method is obtained from $w_i^{(n)} = P(A)w_i^{(0)}$, $i = 1, \ldots, k$, where $P(\mu)$ is a polynomial of some high degree that supresses the unwanted eigenvalues of a hermitian matrix. In particular, $P(\mu)$ is taken to be a Chebyshev polynomial rescaled and shifted to an interval that contains the unwanted eigenvalues. Thus $P(\mu)$ is analogous to our $[\psi(\mu)]^n$. In [19] this approach is extended to non-hermitian matrices. In particular, the polynomial $P(\mu)$ now is taken to be a Chebyshev polynomial rescaled and shifted to an elliptical domain that contains the unwanted eigenvalues. Thus the vector u in the method of Arnoldi is taken to be $u = P(A)u_0$, so that $P(\mu)$ is analogous to our $[\psi(\mu)]^n$ in this case too.

5. Analytical preliminaries

5.1. General considerations

We now begin the investigation of the convergence as $n \to \infty$ of the Ritz values and Ritz vectors for the approach presented in Section 4. Even though we have three different methods, all of these methods can be analyzed within a unified framework as we show below.

The starting point of our investigation is the homogeneous linear system in Eq. (3.4). As mentioned following Eq. (3.4), the Ritz values are the roots of the characteristic equation

$$D_n(\mu) \equiv \det[Y^*Q(\mu I - A)Z] = 0, \tag{5.1}$$

and all our results are obtained by a detailed analysis of this polynomial equation for $n \to \infty$.

Letting $u_{rs}^{(n)}(\mu)$ stand for the (r,s) element of the matrix $Y^*Q(\mu I - A)Z$, $r, s = 1, 2, \ldots, k$, we have for each r and s

$$u_{rs}^{(n)}(\mu) = y_r^* Q(\mu I - A) z_s. \tag{5.2}$$

Note that Eqs. (5.1) and (5.2) are independent of whether A is normal or non-normal, diagonalizable or nondiagonalizable. In the present work, however, we restrict our investigation to normal matrices, as the analytical technique for these matrices is less involved and the actual numerical convergence and the corresponding theoretical results more powerful. We begin this by analyzing the $u_{rs}^{(n)}(\mu)$.

5.2. $u_{rs}^{(n)}(\mu)$ *for normal matrices*

We recall that an $N \times N$ normal matrix A is characterized by the property $A^*A = AA^*$ and has a set of orthonormal eigenvectors that span $\mathbb{C}^N$. The eigenvectors are orthogonal with respect to the standard Euclidean inner product $(a, b) = a^*b$, which we take to be the inner product in the sequel. That is to say, we have $Q = I$ in Eqs. (3.2), (3.4), (5.1), (5.2). In general, this choice of the inner product gives the methods described in the previous section a convergence rate for eigenvalue approximations that is twice as large as that achieved with a different inner product. We will discuss this point further in the next section.

We now give the behavior of the $u_{rs}^{(n)}(\mu)$ for SEA, SEL, and SESI. We assume that

$$\psi(A)v_i = \psi(\mu_i)v_i \quad \text{for all } i, \tag{5.3}$$

which is satisfied, e.g., when $\psi(\mu)$ is a polynomial or a rational function or an exponential function.

(1) $u_{rs}^{(n)}(\mu)$ *for SEA*: Since the vector u_0 has a spectral decomposition of the form $u_0 = \sum_{i=1}^{N} \gamma_i v_i$ for some scalars γ_i, we have

$$u_n = [\psi(A)]^n u_0 = \sum_{i=1}^{N} \gamma_i [\psi(\mu_i)]^n v_i. \tag{5.4}$$

By adding together all the terms that have equal μ_i and $\gamma_i \psi(\mu_i) \neq 0$, and renaming if necessary, we realize that u_n is actually of the form

$$u_n = \sum_{i=1}^{\hat{N}} \gamma_i [\psi(\mu_i)]^n v_i \quad \text{for some } \hat{N} \leqslant N, \tag{5.5}$$

where γ_i, μ_i, and v_i are not necessarily those in Eq. (5.4), and are such that

$$\mu_i \neq \mu_j \quad \text{if } i \neq j, \ \ i, j = 1, \ldots, \hat{N}, \tag{5.6}$$

$$\gamma_i \psi(\mu_i) \neq 0, \quad i = 1, \ldots, \hat{N}, \tag{5.7}$$

and

$$Av_i = \mu_i v_i, \ \ i = 1, \ldots, \hat{N}; \qquad (v_i, v_j) = \delta_{ij}, \ \ i, j = 1, \ldots, \hat{N}. \tag{5.8}$$

Note that Eq. (5.6) means that the μ_i that appear in Eq. (5.5) are *distinct*. The integer $\hat{N}$ is at most equal to the number of the distinct eigenvalues of A, i.e., $\{\mu_1, \mu_2, \ldots, \mu_{\hat{N}}\}$ may be the set of the distinct eigenvalues of A or a proper subset of it.

Combining Eqs. (5.5)–(5.8) with the fact that $y_m = z_m = A^{m-1}u_n$, $m = 1, 2, \ldots, k$, we have

$$y_m = z_m = \sum_{i=1}^{\hat{N}} \gamma_i [\psi(\mu_i)]^n \mu_i^{m-1} v_i, \tag{5.9}$$

so that from Eq. (5.2)

$$u_{rs}^{(n)}(\mu) = \sum_{j=1}^{\hat{N}} \overline{(\gamma_j \mu_j^{r-1})}(\gamma_j \mu_j^{s-1}) |\psi(\mu_j)|^{2n} (\mu - \mu_j). \tag{5.10}$$

(2) $u_{rs}^{(n)}(\mu)$ *for SEL*: The vector $u_n = [\psi(A)]^n u_0$ is obviously precisely the one that was given for SEA. In particular, Eqs. (5.5)–(5.8) hold. Combining this with $z_m = A^{m-1}u_n$ and $y_m = A^{*m-1}u_n$, $m = 1, 2, \ldots, k$, we have

$$z_m = \sum_{i=1}^{\hat{N}} \gamma_i [\psi(\mu_i)]^n \mu_i^{m-1} v_i \quad \text{and} \quad y_m = \sum_{i=1}^{\hat{N}} \gamma_i [\psi(\mu_i)]^n \overline{\mu_i}^{m-1} v_i, \tag{5.11}$$

so that from Eq. (5.2)

$$u_{rs}^{(n)}(\mu) = \sum_{j=1}^{\hat{N}} (\overline{\gamma_j} \mu_j^{r-1})(\gamma_j \mu_j^{s-1}) |\psi(\mu_j)|^{2n} (\mu - \mu_j) \tag{5.12}$$

with the μ_j, the γ_j and $\hat{N}$ being precisely those of Eq. (5.10).

(3) $u_{rs}^{(n)}(\mu)$ *for SESI*: Since the vectors x_m have spectral decompositions $x_m = \sum_{i=1}^{N} \gamma_{mi} v_i$ for some scalars γ_{mi}, we have

$$x_m^{(n)} = [\psi(A)]^n x_m = \sum_{i=1}^{N} \gamma_{mi} [\psi(\mu_i)]^n v_i. \tag{5.13}$$

By excluding the terms for which $\psi(\mu_i) = 0$, and renaming if necessary, we realize that $x_m^{(n)}$ is actually of the form

$$x_m^{(n)} = \sum_{i=1}^{\hat{N}} \gamma_{mi} [\psi(\mu_i)]^n v_i, \quad m = 1, \ldots, k \text{ for some } \hat{N} \leqslant N, \tag{5.14}$$

where γ_{mi}, μ_i, and v_i are not necessarily those in Eq. (5.13) and are such that

$$\psi(\mu_i) \neq 0, \quad i = 1, \ldots, \hat{N} \tag{5.15}$$

and

$$Av_i = \mu_i v_i, \quad i = 1, \ldots, \hat{N}; \qquad (v_i, v_j) = \delta_{ij}, \quad i, j = 1, \ldots, \hat{N}. \tag{5.16}$$

Note that the μ_i in Eq. (5.14) are *not* necessarily distinct. Also, we have the *same* μ_i and v_i for all $m, m = 1, \ldots, k$. Finally, some of the γ_{mi} may be zero. From Eqs. (5.14)–(5.16) and the fact that $y_m = z_m = x_m^{(n)}$, $m = 1, 2, \ldots, k$, and from Eq. (5.2) we have

$$u_{rs}^{(n)}(\mu) = \sum_{j=1}^{\hat{N}} \overline{\gamma_{rj}}\gamma_{sj}|\psi(\mu_j)|^{2n}(\mu - \mu_j). \tag{5.17}$$

Remark 5.1. (i) From Eqs. (5.10), (5.12) and (5.17) we realize that for all the three methods $u_{rs}^{(n)}$ have the *unified* structure

$$u_{rs}^{(n)}(\sigma) = \sum_{j=1}^{M} \beta_{rj}\alpha_{sj}\zeta_j^n(\sigma - \sigma_j), \tag{5.18}$$

so that we have the correspondences $\sigma_j \leftrightarrow \mu_j$ and $\zeta_j \leftrightarrow |\psi(\mu_j)|^2$ and $M \leftrightarrow \hat{N}$ for all the methods. This enables us to analyze them simultaneously.

(ii) Recall that $\mu_1, \mu_2, \ldots, \mu_{\hat{N}}$ in the $u_{rs}^{(n)}(\mu)$ associated with SEA and SEL that are given in Eqs. (5.10) and (5.12), respectively, are some or all of the *distinct* eigenvalues of A. Furthermore, $\gamma_i\psi(\mu_i) \neq 0$, $i = 1, 2, \ldots, \hat{N}$. On the other hand, in the $u_{rs}^{(n)}$ associated with SESI that is given in Eq. (5.17) the μ_i are *not* necessarily distinct. Also, even though $\psi(\mu_i) \neq 0$, $i = 1, \ldots, \hat{N}$, some of the γ_{mi} may be zero. Obviously, $\hat{N}$ in Eqs. (5.10) and (5.12) is not necessarily the same as that in Eq. (5.17).

Now that we have the $u_{rs}^{(n)}$ with the structure in Eq. (5.18), we can use the results of Appendix A to state the main convergence results for Ritz values and vectors.

We preserve the type of ordering given in Eq. (1.1) also after we have renamed the μ_i, i.e., we have the ordering

$$|\psi(\mu_1)| \geqslant |\psi(\mu_2)| \geqslant \cdots \geqslant |\psi(\mu_{\hat{N}})|. \tag{5.19}$$

In the sequel we shall denote $\psi(\mu_i)$ by ψ_i for short.

Finally, all of the above, and, consequently, all of the results in the sequel, hold with no changes also when A is not normal, but the v_i are orthogonal in the sense $v_i^*Qv_j = \delta_{ij}$ with $Q \neq I$ necessarily, cf. Eqs. (5.8) and (5.16).

When A is not normal, and thus the eigenvectors v_i are not all mutually orthogonal, the $u_{rs}^{(n)}$ have expansions that are expressed as double series instead of those given in Eqs. (5.10), (5.12) and (5.17). This makes the analysis of the case of non-normal matrices much more complicated.

6. Analysis of Ritz values for normal matrices

Theorem 6.1 below provides the complete expansion of $D_n(\mu)$ in Eq. (5.1), the polynomial whose zeros are the Ritz values, and plays a central role in the convergence analysis that follows.

Theorem 6.1. *With* $u_{rs}^{(n)}(\mu)$ *as given in* (5.10) *or* (5.12) *or* (5.17), *the polynomial* $D_n(\mu) = \det[u_{rs}^{(n)}(\mu)]_{r,s=1}^{k}$ *has the expansion*

$$D_n(\mu) = \sum_{1 \leq j_1 < j_2 < \cdots < j_k \leq \hat{N}} W_{j_1, j_2, \ldots, j_k} \left[\prod_{p=1}^{k} (\mu - \mu_{j_p})\right] \left(\prod_{p=1}^{k} |\psi_{j_p}|^{2n}\right), \tag{6.1}$$

where

$$W_{j_1, j_2, \ldots, j_k} = \left(\prod_{p=1}^{k} |\gamma_{j_p}|^2\right) |V(\mu_{j_1}, \mu_{j_2}, \ldots, \mu_{j_k})|^2 \quad \textit{for SEA}, \tag{6.2}$$

$$W_{j_1, j_2, \ldots, j_k} = \left(\prod_{p=1}^{k} |\gamma_{j_p}|^2\right) [V(\mu_{j_1}, \mu_{j_2}, \ldots, \mu_{j_k})]^2 \quad \textit{for SEL}, \tag{6.3}$$

and

$$W_{j_1, j_2, \ldots, j_k} = |Z_{j_1, j_2, \ldots, j_k}(\gamma)|^2 \quad \textit{for SESI}. \tag{6.4}$$

Here $\psi_i = \psi(\mu_i)$, $i = 1, 2, \ldots,$ *and* $V(\lambda_1, \lambda_2, \ldots, \lambda_k)$ *is the Vandermonde determinant that is given by*

$$V(\lambda_1, \lambda_2, \ldots, \lambda_k) = \begin{vmatrix} 1 & 1 & \cdots & 1 \\ \lambda_1 & \lambda_2 & \cdots & \lambda_k \\ \lambda_1^2 & \lambda_2^2 & \cdots & \lambda_k^2 \\ \vdots & \vdots & & \vdots \\ \lambda_1^{k-1} & \lambda_2^{k-1} & \cdots & \lambda_k^{k-1} \end{vmatrix} = \prod_{1 \leq i < j \leq k} (\lambda_j - \lambda_i) \tag{6.5}$$

and $Z_{j_1, j_2, \ldots, j_k}(\alpha)$ *is defined in Eq.* (A.7) *of Appendix A.*

Proof. The result follows from Lemma A.2 by making the substitutions $\zeta_j = |\psi_j|^2$, $\sigma_j = \mu_j$ for all three methods, and the substitutions $\alpha_{sj} = \gamma_j \mu_j^{s-1}$ and $\beta_{rj} = \overline{\alpha_{rj}}$ for SEA, $\alpha_{sj} = \gamma_j \mu_j^{s-1}$ and $\beta_{rj} = \overline{\gamma_j} \mu_j^{r-1}$ for SEL, and $\alpha_{sj} = \gamma_{sj}$ and $\beta_{rj} = \overline{\alpha_{rj}}$ for SESI. □

The next theorem provides sufficient conditions for the Ritz values to converge.

Theorem 6.2. *In Theorem* 6.1 *let*

$$|\psi_1| \geqslant |\psi_2| \geqslant \cdots \geqslant |\psi_k| > |\psi_{k+1}| \geqslant \cdots, \tag{6.6}$$

then

$$D_n(\mu) = W_{1,2,\ldots,k}\left(\prod_{j=1}^{k}|\psi_j|^{2n}\right)\left[\prod_{j=1}^{k}(\mu-\mu_j) + \mathrm{O}\left(\left|\frac{\psi_{k+1}}{\psi_k}\right|^{2n}\right)\right]$$
$$\text{as } n \to \infty, \tag{6.7}$$

unconditionally for SEA and SEL, and provided that $Z_{1,2,\ldots,k}(\gamma) \neq 0$ *for SESI. Consequently,* $D_n(\mu)$ *has exactly* k *zeros (the* k *Ritz values) that tend to* $\mu_1, \mu_2, \ldots, \mu_k$.

Proof. The result follows from Lemma A.3 as $W_{1,2,\ldots,k} \neq 0$ for all the three methods. That this is so for SEA and SEL follows from Eqs. (6.2), (6.3), (6.5), (5.6), (5.7), and for SESI it follows from Eq. (6.4) and from the assumption that $Z_{1,2,\ldots,k}(\gamma) \neq 0$. □

Remark 6.1. The condition $Z_{1,2,\ldots,k}(\gamma) \neq 0$ for SESI is equivalent to the requirement that the projections $\sum_{i=1}^{k}\gamma_{mi}v_i$ of the vectors $x_m^{(0)}$, $m = 1,2,\ldots,k$, in Eq. (5.14) unto the subspace span $\{v_1, v_2, \ldots, v_k\}$ be linearly independent. This can be seen by using Eq. (A.7).

Theorem 6.3. *Assume that the conditions of Theorem* 6.2 *hold, and denote the Ritz value that tends to* μ_s *by* $\mu_s(n)$, $s = 1,2,\ldots,k$. *Then*

$$\mu_s(n) = \mu_s + \mathrm{O}\left(\left|\frac{\psi_{k+1}}{\psi_s}\right|^{2n}\right) \quad \text{as } n \to \infty \tag{6.8}$$

for all three methods. For SEA and SEL and, provided $\mu_s \neq \mu_j$ *for* $s \neq j$, *for SESI as well, this result can be refined in an optimal way as follows: Let* r *be the integer for which*

$$|\psi_k| > |\psi_{k+1}| = \cdots = |\psi_{k+r}| > |\psi_{k+r+1}|. \tag{6.9}$$

Then

$$\mu_s(n) \sim \mu_s + K_s\left|\frac{\psi_{k+1}}{\psi_s}\right|^{2n} \quad \text{as } n \to \infty, \tag{6.10}$$

where K_s *is a constant given by*

$$K_s = \sum_{i=1}^{r}\left|\frac{\gamma_{k+i}}{\gamma_s}\right|^2\left(\prod_{\substack{j=1\\ j\neq s}}^{k}\left|\frac{\mu_{k+i}-\mu_j}{\mu_s-\mu_j}\right|^2\right)(\mu_{k+i}-\mu_s) \quad \textit{for SEA}, \tag{6.11}$$

$$K_s = \sum_{i=1}^{r} \left| \frac{\gamma_{k+i}}{\gamma_s} \right|^2 \left(\prod_{\substack{j=1 \\ j \neq s}}^{k} \frac{\mu_{k+i} - \mu_j}{\mu_s - \mu_j} \right)^2 (\mu_{k+i} - \mu_s) \quad \textit{for SEL} \tag{6.12}$$

and

$$K_s = \sum_{i=1}^{r} \left| \frac{Z_{1,2,\ldots,s-1,s+1,\ldots,k,k+i}}{Z_{1,2,\ldots,k}} \right|^2 (\mu_{k+i} - \mu_s) \quad \textit{for SESI}. \tag{6.13}$$

Proof. The proof of this theorem is established by using Lemma A.5 along with Eqs. (6.2)–(6.4). □

It is interesting to note that when $\mu_s \neq \mu_j$ for $s \neq j$, the Ritz value $\mu_s(n)$ tends to μ_s *monotonically* along a ray that makes an angle of arg K_s with the real axis.

We mention that the result of Theorem 6.3 with $\psi(\mu) = \mu$ was originally given in [20] for the method of Arnoldi and in [22] for the method of Lanczos. Again with $\psi(\mu) = \mu$ and for hermitian matrices a slightly weaker form of Eq. (6.8), namely,

$$\limsup_{n\to\infty} |\mu_s(n) - \mu_s|^{1/n} \leqslant \left| \frac{\psi_{k+1}}{\psi_s} \right|^2$$

was given for the simultaneous iteration method in [25].

Before closing this section we note that when A is not normal, the results of Theorems 6.2 and 6.3 are modified substantially. Thus, subject to Eq. (6.6), the result of Eq. (6.7) is replaced by

$$D_n(\mu) = W \left(\prod_{j=1}^{k} |\psi_j|^{2n} \right) \left[\prod_{j=1}^{k} (\mu - \mu_j) + \mathrm{O}\left(\left| \frac{\psi_{k+1}}{\psi_k} \right|^n \right) \right] \quad \text{as } n \to \infty$$

for some nonzero constant W, while the result in Eq. (6.8) is replaced by

$$\mu_s(n) = \mu_s + \mathrm{O}\left(\left| \frac{\psi_{k+1}}{\psi_s} \right|^n \right) \quad \text{as } n \to \infty,$$

and this shows that better accuracy is produced for normal matrices. As mentioned earlier, the proofs of these results are more complicated than the ones we have given in the present work, and they will be the subject of a future publication.

Finally, we note also that in any case the approximations for μ_1 are the best, followed by those for $\mu_2, \mu_3, \ldots, \mu_k$, in this order.

7. Analysis of Ritz vectors for normal matrices

We now analyze the convergence behavior of the Ritz vectors. Denote by $v_s(n)$ the Ritz vector that corresponds to the Ritz value $\mu_s(n)$. If we let the eigenvector of the matrix pencil (Y^*AZ, Y^*Z) that corresponds to $\mu_s(n)$ be $\xi_s(n) = (\xi_{s1}(n), \ldots, \xi_{sk}(n))^T$, then we have

$$v_s(n) = z\xi_s(n) = \sum_{i=1}^{k} \xi_{si}(n) z_i. \tag{7.1}$$

Invoking in Eq. (7.1) the expressions for z_i that we gave in Section 5 for the three methods, we obtain the spectral decomposition

$$v_s(n) = \sum_{j=1}^{\hat{N}} \delta_{sj}(n) \psi_j^n v_j, \tag{7.2}$$

where

$$\delta_{sj}(n) = \sum_{i=1}^{k} \alpha_{ij} \xi_{si}(n), \tag{7.3}$$

with $\alpha_{ij} = \gamma_i \mu_i^{j-1}$ for SEA and SEL, and $\alpha_{ij} = \gamma_{ij}$ for SESI. In fact, α_{ij} are exactly the ones that appear in $u_{rs}^{(n)}(n) = \sum_{j=1}^{\hat{N}} \beta_{rj}\alpha_{sj}|\psi_j|^{2n}(\mu - \mu_j)$. Thus we see that if we know the behavior of the $\delta_{sj}(n)$ for $n \to \infty$, then we can determine that of $v_s(n)$ as well. This is precisely the approach that we take to this question in Theorem 7.1 below. While for SEA and SEL we have no additional assumptions, for SESI we assume that $\mu_s \neq \mu_j$ for $s \neq j$ in Eq. (5.14).

Theorem 7.1. *Assume that the conditions of Theorem* 6.2 *hold. Then, with proper normalization of the vector* $\xi_s(n)$, *the* $\delta_{sj}(n)$ *satisfy*

$$\delta_{sj}(n) = \begin{cases} \mathrm{O}(1) & \text{for } j \geq k+1, \\ 1 + \mathrm{o}(1) & \text{for } j = s, \\ \mathrm{O}(\psi_{k+1}^{2n}\psi_j^{-2n}) & \text{for } 1 \leq j \leq k,\ j \neq s,\ \text{as } n \to \infty. \end{cases} \tag{7.4}$$

Consequently, the Ritz vector $v_s(n)$, *when normalized suitably, satisfies*

$$v_s(n) = v_s + \sum_{\substack{j=1 \\ j\neq s}}^{\hat{N}} \epsilon_{sj}(n) v_j \tag{7.5}$$

with

$$\epsilon_{sj}(n) = \begin{cases} \mathrm{O}(\psi_j^n \psi_s^{-n}) & \text{for } j \geq k+1, \\ \mathrm{O}(\psi_{k+1}^{2n}\psi_j^{-n}\psi_s^{-n}) & \text{for } 1 \leq j \leq k,\ j \neq s,\ \text{as } n \to \infty. \end{cases} \tag{7.6}$$

which implies that

$$v_s(n) = v_s + \mathrm{O}\left(\left|\frac{\psi_{k+1}}{\psi_s}\right|^n\right) \quad \text{as } n \to \infty. \tag{7.7}$$

Proof. First, we recall that the $\xi_{si}(n)$ are the solution to the homogeneous system of equations in Eq. (3.4), i.e., they satisfy

$$\sum_{i=1}^{k} u_{ri}^{(n)}(\mu_s(n))\xi_{si}(n) = 0, \quad 1 \leqslant r \leqslant k. \tag{7.8}$$

Noting the similarity of Eq. (7.8) with Eq. (A.39) and of Eq. (7.3) with Eq. (A.40), we see that Lemma A.6 applies. This results in Eq. (7.4). The rest is a direct outcome of Eqs. (7.2) and (7.4). □

With $\psi(\mu) = \mu$ and for hermitian matrices, a slightly weaker form of Eq. (7.7), namely

$$\limsup_{n\to\infty} \|v_s(n) - v_s\|^{1/n} \leqslant \left|\frac{\psi_{k+1}}{\psi_s}\right|,$$

was given for the simultaneous iteration method in [25].

We know that $(v_i, v_j) = 0$ when $i \neq j$. An immediate question of interest that arises in connection with Ritz vectors is that of how close $(v_r(n), v_s(n))$ is to zero when $r \neq s$. We provide the answer to this question in Theorem 7.2 below.

Theorem 7.2. *Let $v_r(n)$ and $v_s(n)$ be two Ritz vectors that correspond to the Ritz values $\mu_r(n)$ and $\mu_s(n)$, respectively. Assume that they have been normalized such that $(v_i(n), v_i(n)) = 1$, $i = r, s$. Then, under the conditions of Theorem* 6.2,

$$(v_r(n), v_s(n)) = \mathrm{O}\left(\left|\frac{\psi_{k+1}}{\psi_r}\right|^n \left|\frac{\psi_{k+1}}{\psi_s}\right|^n\right) \quad \text{as } n \to \infty \tag{7.9}$$

for SEA and SEL, and, provided $\mu_r, \mu_s \neq \mu_j$ for $j \neq r, s$ in Eq. (5.14), *for SESI as well.*

Proof. The result follows from Eqs. (7.5) and (7.6). □

We note that the result in Eq. (7.9) for the simultaneous iteration method when $\psi(\mu) = \mu$ can be found, for example, in [14]. Again, as will be shown in a future publication, subject to Eq. (6.6), the result of Eq. (7.7) remains unchanged when A is not normal.

8. Formation of spurious approximate eigenvalues

An important requirement that makes the results of Theorems 6.2, 6.3, 7.1, and 7.2 possible is the condition $|\psi_k| > |\psi_{k+1}|$ in Eq. (6.6). In the absence of this condition, namely, when $|\psi_k| = |\psi_{k+1}|$, the proofs of these theorems are no longer valid. In this section we provide new versions for Theorems 6.2 and 6.3 that concern $D_n(\mu)$ and its zeros under the new condition $|\psi_k| = |\psi_{k+1}|$.

One of the consequences of $|\psi_k| = |\psi_{k+1}|$ is that some of the Ritz values are approximations to a number of the eigenvalues $\mu_1, \mu_2, \ldots$, in this order, while the rest are spurious approximations that depend on the α_{rj} and, generally, have nothing to do with the spectrum of A.

Theorem 8.1. *In Theorem* 6.1 *let*

$$|\psi_1| \geqslant \cdots \geqslant |\psi_t| > |\psi_{t+1}| = \cdots = |\psi_{t+r}| > |\psi_{t+r+1}| \geqslant \cdots \tag{8.1}$$

for some $t \geqslant 0$ *and* $r \geqslant 2$, *and let*

$$t + 1 \leqslant k < t + r. \tag{8.2}$$

Define

$$S(\mu) = \sum_{t+1 \leqslant j_{t+1} < \cdots < j_k \leqslant t+r} W_{1,2,\ldots,t,j_{t+1},\ldots,j_k} \left[\prod_{p=t+1}^{k} (\mu - \mu_{j_p}) \right] \tag{8.3}$$

with $W_{j_1,j_2,\ldots,j_k}$ *as defined by Eqs.* (6.2)–(6.4) *for the three methods. Assume that*

$$Z_{1,2,\ldots,t,j_{t+1},\ldots,j_k}(\gamma) \neq 0 \quad \text{for some } j_{t+1}, \ldots, j_k \text{ in Eq. (8.3) for SESI} \tag{8.4}$$

and

$$\sum_{t+1 \leqslant j_{t+1} < \cdots < j_k \leqslant t+r} W_{1,2,\ldots,t,j_{t+1},\ldots,j_k} \neq 0 \quad \text{for SEL}, \tag{8.5}$$

while no additional assumption is needed for SEA. Thus $S(\mu)$ *is a polynomial in* μ *of degree exactly* $q = k - t$. *Denote the zeros of* $S(\mu)$ *by* $\mu'_1, \ldots, \mu'_q$. *Then*

$$d_n D_n(\mu) = \prod_{j=1}^{t} (\mu - \mu_j) \prod_{j=1}^{q} (\mu - \mu'_j) + O(\epsilon_t^{2n}) \quad \text{as } n \to \infty, \tag{8.6}$$

where d_n *is an appropriate constant and*

$$\epsilon_t = \max \left(\left| \frac{\psi_{t+1}}{\psi_t} \right|, \left| \frac{\psi_{t+r+1}}{\psi_{t+r}} \right| \right). \tag{8.7}$$

Consequently, $D_n(\mu)$ *has* t *Ritz values* $\mu_1(n), \ldots, \mu_t(n)$ *that tend to* $\mu_1, \ldots, \mu_t$, *and* q *others that tend to* $\mu'_1, \ldots, \mu'_q$.

When $\mu_s \notin \{\mu'_1, \ldots, \mu'_q\}$ *and* $1 \leqslant s \leqslant t$, *we have*

$$\mu_s(n) = \mu_s + O\left(\left|\frac{\psi_{t+1}}{\psi_s}\right|^{2n}\right) \quad \text{as } n \to \infty \tag{8.8}$$

for all three methods.

Proof. The proof of Eqs. (8.6) and (8.7) can be accomplished by employing Lemma A.7, while that of Eq. (8.8) follows from Lemma A.8. □

We must note that the spurious eigenvalue approximations mentioned in Theorem 8.1 should be present theoretically, i.e., in exact arithmetic, under the condition $|\psi_k| = |\psi_{k+1}|$. They, therefore, do not seem to have much in common with the "spurious" or "ghost" eigenvalues that appear in applications of the method of Lanczos in finite precision arithmetic.

9. Numerical examples

Consider the $N \times N$ matrix $A = \text{tridiag}\,(\rho, 0, \tau)$, where ρ and τ are real. The eigenvalues of this matrix are

$$2\sqrt{\rho\tau}\cos\frac{j\pi}{N+1}, \quad j = 1, \ldots, N.$$

For the sake of simplicity we pick ρ and τ such that $2\sqrt{\rho\tau} = 1$ so that the spectrum of A lies in $(-1, 1)$.

Suppose now that we are interested in the eigenvalues that are closest to 0. For this we need to pick a function $\psi(\mu)$ that is largest in a neighborhood of $\mu = 0$ for $\mu \in (-1, 1)$. A simple yet effective choice would be $\psi(\mu) = a^2 - \mu^2$ with $a^2 > \frac{1}{2}$, so that $|\psi(0)| > |\psi(\mu)|$ for all $\mu \in (-1, 1) \setminus \{0\}$. Note that this choice is also quite inexpensive as it involves only two matrix–vector multiplications in the computation of $\psi(A)u = a^2u - A(Au)$.

Unless there is strong clustering of eigenvalues about 0, the methods SEA, SEL, and SESI are expected to produce good approximations for the eigenvalues of A that are in the immediate neighborhood of 0. Depending on the value of the integer n (in u_n) and on the size of the rounding unit of the floating point arithmetic being used, eigenvalues μ_i for which $|\psi(\mu_i)/\psi(\mu_1)|^n$ is less than the rounding unit are not expected to be approximated well. The reason for this is that the contributions $\gamma_i[\psi(\mu_i)]^n v_i$ for such μ_i are not noticeable *numerically* in u_n, cf. Eq. (5.4), if we assume that the γ_i are all of comparable sizes. (As we normally pick u_0 randomly, this assumption is quite reasonable.)

We have done numerical computations for various values of N, ρ, τ, a, and n. All the computations have been carried out in double precision arithmetic (approximately 14 decimal digits). The method that has been used is SEA, the vector u_0 being random.

In Tables 1 and 2 we show some of the numerical results obtained for the following two cases:

(i) $N = 51$ and $\rho = \tau = 1/2$. (A is real symmetric, hence normal, in this case.)

(ii) $N = 51, \rho = 1/2.2$, and $\tau = 0.55$. (A is not normal for this case.)

We also picked $a = 0.8$, $n = 100$, and $u_0 = (1, 1/\sqrt{2}, \ldots, 1/\sqrt{N})^{\mathrm{T}}$.

For both cases 0 is an eigenvalue and the spectra are symmetric with respect to 0. We expect to obtain good approximations to the eigenvalue $\mu_1 = 0$ and to a number of eigenvalues closest to it. From our discussion in the second paragraph of this section we do not expect to be able to approximate those eigenvalues μ_i that satisfy

$$|\psi(\mu_i)/\psi(\mu_1)|^n = |(a^2 - \mu_i^2)/a^2|^n \underset{\sim}{<} 10^{-14}.$$

With a and n picked as above, this implies that the eigenvalues μ_i for which

$$|\mu_i| \underset{\sim}{>} \sqrt{a^2(1 - 10^{-14/n})} = \sqrt{0.8(1 - 10^{-0.14})} = 0.469\cdots$$

cannot be approximated. Thus, we expect to approximate the eigenvalues $0, \pm 0.0604, \pm 0.121, \pm 0.180, \pm 0.239, \pm 0.298, \pm 0.355, \pm 0.410$ (rounded to 3 decimal digits), but not the rest of the eigenvalues, beginning with ± 0.465 (rounded to 3 decimal digits, again). Again, from our theory we expect to obtain the best approximations for $\mu_1 = 0$, followed by those for $\pm 0.0604, \pm 0.121$, etc. To a large extent, all these expectations seem to be verified by our numerical experiments as Tables 1 and 2 show. Recall also that the Ritz values for $k = 1$ are the ones obtained from the generalized power method described in Theorem 2.1.

10. Concluding remarks

In this work we have described an approach by which one can employ known Krylov subspace methods to obtain approximations to eigenvalues of a matrix that have special properties. In particular, we have considered the methods of Arnoldi and Lanczos and the simultaneous iteration method, and have provided a detailed analysis of convergence for them as they are applied to normal matrices and stated without proofs the corresponding results for non-normal matrices. From the theory of convergence it follows that when the matrix A has eigenvalues of multiplicity 1, all three methods produce the same rates of convergence. When A has eigenvalues of multiplicity 2 or more, however, the Arnoldi and Lanczos methods have better convergence properties. The reason for this is that the Arnoldi and Lanczos methods produce at most one Ritz value for a multiple eigenvalue, and also one Ritz vector for a corresponding eigenvector. The simultaneous iteration method, on the other hand, will produce a number of Ritz values for a multiple eigenvalue, this number being equal to the multiplicity of the eigenvalue in general. In addition, it

Table 1
Absolute errors in the Ritz values obtained from SEA applied to the $N \times N$ matrix $A = \text{tridiag}\ (\rho, 0, \tau)$, with $N = 51, \rho = \tau = 1/2$, beginning with the vector $u_n = [\psi(A)]^n u_0$, where $\psi(\mu) = 0.8 - \mu^2, u_0 = (1, 1/\sqrt{2}, ..., 1/\sqrt{N})^T$, and $n = 100$ (here k is the dimension of the relevant Krylov subspace)

μ_i	$k=1$	$k=3$	$k=5$	$k=7$	$k=9$	$k=11$	$k=13$	$k=15$	$k=17$	$k=19$
−0.465									5.10 D−01	4.49 D−01
−0.410								3.02 D−01	7.54 D−03	7.92 D−05
−0.355							1.61 D−05	1.44 D−05	2.14 D−06	2.25 D−08
−0.298						5.65 D−05	7.33 D−09	6.90 D−09	7.61 D−10	6.86 D−12
−0.239					7.49 D−04	3.36 D−07	4.77 D−13	1.23 D−11	1.91 D−12	1.61 D−14
−0.180				1.61 D−03	8.96 D−06	3.44 D−10	2.58 D−13	3.89 D−14	7.66 D−15	1.39 D−16
−0.121			1.10 D−02	1.57 D−04	4.19 D−07	3.54 D−10	2.94 D−14	8.44 D−15	4.72 D−16	2.64 D−16
−0.0604		1.00 D−02	8.91 D−04	2.09 D−05	2.51 D−07	7.11 D−11	3.86 D−15	1.19 D−15	1.94 D−16	5.55 D−17
0	3.75 D−03	4.07 D−03	1.75 D−03	6.55 D−05	3.66 D−07	8.05 D−11	4.04 D−15	1.51 D−15	1.16 D−16	1.63 D−16
0.0604		1.53 D−02	3.38 D−03	9.99 D−05	5.27 D−07	1.15 D−10	5.50 D−15	2.05 D−15	4.86 D−17	4.86 D−17
0.121			1.60 D−02	6.22 D−04	4.38 D−06	1.15 D−09	6.29 D−14	2.52 D−14	2.50 D−16	9.71 D−17
0.180				2.50 D−03	3.61 D−05	1.46 D−08	1.05 D−12	4.69 D−13	4.97 D−15	1.39 D−16
0.239					1.29 D−03	1.22 D−06	1.44 D−10	7.31 D−11	1.06 D−12	7.36 D−15
0.298						8.83 D−05	2.59 D−08	1.56 D−08	3.26 D−10	2.53 D−12
0.355							2.82 D−05	2.12 D−05	8.11 D−07	7.20 D−09
0.410								1.87 D−01	1.96 D−03	1.94 D−05
0.465									5.08 D−01	4.49 D−01

Table 2
Absolute errors in the Ritz values obtained from SEA applied to the $N \times N$ matrix A = tridiag $(\rho, 0, \tau)$, with $N = 51$, $\rho = 1/2.2$, and $\tau = 0.55$, beginning with the vector $u_n = [\psi(A)]^n u_0$, where $\psi(\mu) = 0.8 - \mu^2$, $u_0 = (1, 1/\sqrt{2}, ..., 1/\sqrt{N})^T$, and $n = 100$ (here k is the dimension of the relevant Krylov subspace)

μ_i	$k=1$	$k=3$	$k=5$	$k=7$	$k=9$	$k=11$	$k=13$	$k=15$	$k=17$	$k=19$
−0.465									5.18 D−01	5.02 D−01
−0.410								2.21 D−01	9.87 D−04	5.59 D−04
−0.355							2.10 D−03	1.76 D−03	4.62 D−05	1.03 D−05
−0.298						4.52 D−03	8.70 D−05	6.52 D−05	1.05 D−06	1.57 D−07
−0.239					1.83 D−02	6.34 D−04	4.60 D−06	3.28 D−06	4.40 D−08	5.01 D−09
−0.180				3.93 D−02	4.96 D−03	2.52 D−07	5.24 D−05	1.85 D−07	2.43 D−09	2.05 D−10
−0.121			7.60 D−02	2.65 D−02	8.08 D−04	6.67 D−06	2.15 D−08	2.12 D−08	3.48 D−10	1.25 D−11
−0.0604		3.73 D−02	5.59 D−02	1.76 D−03	7.68 D−05	1.29 D−07	3.55 D−09	1.42 D−09	7.36 D−11	3.19 D−12
0	1.32 D−02	5.82 D−02	6.73 D−02	3.41 D−03	1.44 D−04	2.09 D−06	1.11 D−08	2.79 D−09	4.10 D−11	7.81 D−12
0.0604		7.40 D−02	4.63 D−02	7.45 D−03	3.93 D−04	4.72 D−06	2.29 D−08	8.04 D−09	3.34 D−11	1.60 D−11
0.121			4.94 D−02	3.31 D−02	1.47 D−03	1.95 D−05	1.00 D−07	4.03 D−08	6.70 D−11	7.44 D−11
0.180				4.31 D−02	7.26 D−03	9.45 D−05	5.78 D−07	2.60 D−07	1.77 D−10	5.04 D−10
0.239					2.17 D−02	8.93 D−04	7.59 D−06	3.85 D−06	8.77 D−10	8.56 D−09
0.298						5.38 D−03	1.18 D−04	6.99 D−05	1.63 D−08	2.14 D−07
0.355							2.38 D−03	1.75 D−03	2.97 D−06	1.17 D−05
0.410								1.35 D−01	3.49 D−04	5.62 D−04
0.465									5.18 D−01	5.01 D−01

will produce the same number of Ritz vectors for the corresponding eigenvectors.

Acknowledgements

This research was carried out in part at NASA Lewis Research Center, Cleveland, Ohio and was supported by a Summer Faculty Fellowship from the Ohio Aerospace Institute. It was also supported in part by the Fund for the Promotion of Research at the Technion.

Appendix A

A.1. General considerations

The purpose of this appendix is to provide the mathematical tools that are used in analyzing the polynomials $D_n(\mu)$ and their zeros in the limit as $n \to \infty$. We believe that the results which we obtain here are of interest in themselves as the techniques used in obtaining them are rather general and may apply to other problems as well.

Lemma A.1. *Let $i_1, \ldots, i_k$ be positive integers, and assume that the scalars $v_{i_1,\ldots,i_k}$ are odd under an interchange of any two indices $i_1, \ldots, i_k$. Let $t_{i,j}$, $i \geqslant 1$, $1 \leqslant j \leqslant k$, be scalars. Define*

$$I_{k,N} = \sum_{i_1=1}^{N} \cdots \sum_{i_k=1}^{N} \left(\prod_{p=1}^{k} t_{i_p,p} \right) v_{i_1,\ldots,i_k} \tag{A.1}$$

and

$$J_{k,N} = \sum_{1 \leqslant i_1 < i_2 < \cdots < i_k \leqslant N} \begin{vmatrix} t_{i_1,1} & t_{i_2,1} & \cdots & t_{i_k,1} \\ t_{i_1,2} & t_{i_2,2} & \cdots & t_{i_k,2} \\ \vdots & \vdots & & \vdots \\ t_{i_1,k} & t_{i_2,k} & \cdots & t_{i_k,k} \end{vmatrix} v_{i_1,\ldots,i_k}. \tag{A.2}$$

Then

$$I_{k,N} = J_{k,N}. \tag{A.3}$$

This lemma was stated and proved in [24]. Lemmas A.2–A.4 below are analogous to Lemmas 2.2 and 2.3 in [20]. For simplicity of notation below we shall use the shorthand notation

$$\sum_{j}, \quad \sum_{j_1<j_2<\cdots<j_k}, \quad \alpha_n \sim \beta_n$$

to mean, respectively,

$$\sum_{j=1}^{\infty}, \quad \sum_{j_1=1}^{\infty}\sum_{j_2=j_1+1}^{\infty}\cdots\sum_{j_k=j_{k-1}+1}^{\infty}, \quad \alpha_n \sim \beta_n \text{ as } n \to \infty.$$

We note that the polynomial $H_n(\sigma)$ that is defined in Lemma A.2 and analyzed throughout is a generalization of the polynomial $D_n(\mu)$. Consequently, all of the results that we prove for $H_n(\sigma)$, after the proper analogy is drawn, are good for $D_n(\mu)$ as well.

Lemma A.2. *Let $\sigma_1, \sigma_2, \ldots$, and $\zeta_1, \zeta_2, \ldots$, be two sequences of complex numbers, and*

$$|\zeta_1| \geqslant |\zeta_2| \geqslant |\zeta_3| \geqslant \cdots; \ \zeta_j \neq 0, \quad j = 0, 1, \ldots, \tag{A.4}$$

and assume that there can be only a finite number of ζ_j's having the same modulus. Let $H_n(\sigma)$ be a polynomial in σ of degree k defined by

$$H_n(\sigma) = \begin{vmatrix} u_{11}^{(n)}(\sigma) & u_{12}^{(n)}(\sigma) & \cdots & u_{1k}^{(n)}(\sigma) \\ u_{21}^{(n)}(\sigma) & u_{22}^{(n)}(\sigma) & \cdots & u_{2k}^{(n)}(\sigma) \\ \vdots & \vdots & & \vdots \\ u_{k1}^{(n)}(\sigma) & u_{k2}^{(n)}(\sigma) & \cdots & u_{kk}^{(n)}(\sigma) \end{vmatrix}, \tag{A.5}$$

where

$$u_{rs}^{(n)}(\sigma) \sim \sum_{j=1}^{\infty} \beta_{rj}\alpha_{sj}\zeta_j^n(\sigma - \sigma_j) \quad \text{as } n \to \infty. \tag{A.6}$$

Define the scalars

$$Z_{j_1,j_2,\ldots,j_k}(\alpha) = \begin{vmatrix} \alpha_{1j_1} & \alpha_{2j_1} & \cdots & \alpha_{kj_1} \\ \alpha_{1j_2} & \alpha_{2j_2} & \cdots & \alpha_{kj_2} \\ \vdots & \vdots & & \vdots \\ \alpha_{1j_k} & \alpha_{2j_k} & \cdots & \alpha_{kj_k} \end{vmatrix} \tag{A.7}$$

with $j_1, \ldots, j_k$ being positive integers. Define the scalars $Z_{j_1,j_2,\ldots,j_k}(\beta)$ similarly, and set

$$W_{j_1,j_2,\ldots,j_k} = Z_{j_1,j_2,\ldots,j_k}(\alpha)Z_{j_1,j_2,\ldots,j_k}(\beta). \tag{A.8}$$

Then we have

$$H_n(\sigma) \sim \sum_{j_1<j_2<\cdots<j_k} W_{j_1,j_2,\ldots,j_k} \left[\prod_{p=1}^{k}(\sigma-\sigma_{j_p})\right]\left(\prod_{p=1}^{k}\zeta_{j_p}^n\right). \tag{A.9}$$

(*If the summation in Eq.* (A.6) *is finite, and* $\sim$ *is replaced by* $=$, *then the multiple sum in Eq.* (A.9) *is finite, and* $\sim$ *is replaced by* $=$ *there too.*)

Proof. Substituting Eq. (A.6) in Eq. (A.5), we obtain

$$H_n(\sigma) \sim \begin{vmatrix} \sum_{j_1}\beta_{1j_1}\alpha_{1j_1}\zeta_{j_1}^n(\sigma-\sigma_{j_1}) & \sum_{j_1}\beta_{1j_1}\alpha_{2j_1}\zeta_{j_1}^n(\sigma-\sigma_{j_1}) & \cdots & \sum_{j_1}\beta_{1j_1}\alpha_{kj_1}\zeta_{j_1}^n(\sigma-\sigma_{j_1}) \\ \sum_{j_2}\beta_{2j_2}\alpha_{1j_2}\zeta_{j_2}^n(\sigma-\sigma_{j_2}) & \sum_{j_2}\beta_{2j_2}\alpha_{2j_2}\zeta_{j_2}^n(\sigma-\sigma_{j_2}) & \cdots & \sum_{j_2}\beta_{2j_2}\alpha_{kj_2}\zeta_{j_2}^n(\sigma-\sigma_{j_2}) \\ \vdots & \vdots & & \vdots \\ \sum_{j_k}\beta_{kj_k}\alpha_{1j_k}\zeta_{j_k}^n(\sigma-\sigma_{j_k}) & \sum_{j_k}\beta_{kj_k}\alpha_{2j_k}\zeta_{j_k}^n(\sigma-\sigma_{j_k}) & \cdots & \sum_{j_k}\beta_{kj_k}\alpha_{kj_k}\zeta_{j_k}^n(\sigma-\sigma_{j_k}) \end{vmatrix}. \tag{A.10}$$

Using the multilinearity property of determinants, and removing common factors from each row, we can express Eq. (A.10) in the form

$$H_n(\sigma) \sim \sum_{j_1}\sum_{j_2}\cdots\sum_{j_k}\left(\prod_{p=1}^{k}\beta_{pj_p}\right)\left(\prod_{p=1}^{k}\zeta_{j_p}^n\right)\left[\prod_{p=1}^{k}(\sigma-\sigma_{j_p})\right]Z_{j_1,j_2,\ldots,j_k}(\alpha). \tag{A.11}$$

Since the product $\left(\prod_{p=1}^{k}\zeta_{j_p}^n\right)\left[\prod_{p=1}^{k}(\sigma-\sigma_{j_p})\right]Z_{j_1,j_2,\ldots,j_k}(\alpha)$ in Eq. (A.11) is odd under an interchange of any two of the indices $j_1,\ldots,j_k$, Lemma A.1 applies, and Eq. (A.9) follows. □

A.2. Analysis of the zeros of $H_n(\sigma)$ *when* $|\zeta_k| > |\zeta_{k+1}|$

We now start the analysis of the zeros of $H_n(\sigma)$. We show that, under appropriate conditions, the zeros of $H_n(\sigma)$ tend to $\sigma_1,\ldots,\sigma_k$ as $n\to\infty$. We also provide the precise rates of convergence.

Lemma A.3. *If in Lemma* A.2 *we also assume that*

$$|\zeta_k| > |\zeta_{k+1}| \tag{A.12}$$

and

$$W_{1,2,\ldots,k} \neq 0, \tag{A.13}$$

then, for $\sigma \neq \sigma_i$, $1 \leqslant i \leqslant k$, *the dominant behavior of* $H_n(\sigma)$ *is given by*

$$H_n(\sigma) = W_{1,2,\ldots,k}\left(\prod_{j=1}^{k}\zeta_j^n\right)\left[\prod_{j=1}^{k}(\sigma-\sigma_j) + \mathrm{O}\left(\left|\frac{\zeta_{k+1}}{\zeta_k}\right|^n\right)\right] \quad \text{as } n\to\infty. \tag{A.14}$$

This implies that $H_n(\sigma)$ has precisely k zeros that tend to $\sigma_1,\sigma_2,\ldots,\sigma_k$ as $n\to\infty$.

Proof. By Eqs. (A.12) and (A.13) the dominant term in Eq. (A.9) is that for which $j_1=1, j_2=2,\ldots,j_k=k$, this term being of order $|\zeta_1\zeta_2\cdots\zeta_k|^n$. The next dominant terms are of order $|\zeta_1\zeta_2\cdots\zeta_{k-1}\zeta_{k+1}|^n$ by the assumption that there can be only a finite number of ζ_j's having modulus equal to $|\zeta_{k+1}|$. By this Eq. (A.14) now follows. □

Definition A.1. Let s be an integer in $\{1,2,\ldots,k\}$. We shall say that σ_s has multiplicity ω if the set $\{\sigma_1,\sigma_2,\ldots,\sigma_k\}$ contains precisely ω elements that are equal to σ_s, including σ_s itself. If $\omega=1$, we shall say that σ_s is simple, otherwise, we say that it is multiple. In case σ_s has multiplicity $\omega>1$, we shall also assume that $\sigma_s=\sigma_{s+1}=\cdots=\sigma_{s+\omega-1}$ and $|\zeta_s|=|\zeta_{s+1}|=\cdots=|\zeta_{s+\omega-1}|$, as happens in eigenvalue problems.

Now by Lemma A.3 the zeros $\sigma_1(n),\ldots,\sigma_k(n)$ of $H_n(\sigma)$ tend to $\sigma_1,\ldots,\sigma_k$ as $n\to\infty$, whether the latter are simple or multiple. The rates of convergence, however, depend entirely on the σ_j but not on their multiplicities as we show in Lemma A.4. Before going into this lemma, however, we wish to present a perturbation lemma concerning the zeros of certain polynomials, which is of interest in itself. We note that Lemma 2.5 in [21] is similar in spirit to the perturbation lemma we are about to state, although its results are rather different.

Lemma A.4. *Let the polynomial $\Phi_n(\sigma)$ be given by*

$$\Phi_n(\sigma) = \sum_{i=0}^{k} d_i(n)(\sigma-\hat{\sigma})^i \quad \text{for some fixed } \hat{\sigma}, \tag{A.15}$$

such that

$$\lim_{n\to\infty}\frac{d_i(n)}{d_\omega(n)} = \begin{cases} 0 & \text{for } 0\leqslant i\leqslant \omega-1,\\ \hat{d}_i & \text{for } \omega\leqslant i\leqslant k.\end{cases} \tag{A.16}$$

1. *$\Phi_n(\sigma)$ has precisely ω zeros $\hat{\sigma}_l(n)$, $1\leqslant l\leqslant\omega$, that tend to $\hat{\sigma}$ as $n\to\infty$.*
2. *If $\omega=1$, then the unique zero $\hat{\sigma}_1(n)$ of $\Phi_n(\sigma)$ that tends to $\hat{\sigma}$ satisfies precisely*

$$\hat{\sigma}_1(n) \sim \hat{\sigma} - \frac{d_0(n)}{d_1(n)} \quad \text{as } n\to\infty. \tag{A.17}$$

3. *For any $\omega\geqslant 1$ assume that the $d_i(n)$ satisfy*

$$\frac{d_i(n)}{d_\omega(n)} = \mathrm{O}((\epsilon_1\epsilon_2\cdots\epsilon_{\omega-i})^n) \quad \text{as } n \to \infty,\ 0 \leqslant i \leqslant \omega - 1, \tag{A.18}$$

where

$$1 > \epsilon_1 \geqslant \epsilon_2 \geqslant \cdots \geqslant \epsilon_\omega \geqslant 0. \tag{A.19}$$

Then,

$$\hat{\sigma}_l(n) = \hat{\sigma} + \mathrm{O}(\epsilon_1^n) \quad \text{as } n \to \infty,\ 1 \leqslant l \leqslant \omega. \tag{A.20}$$

Proof. The proof of part (1) is obvious from

$$\lim_{n\to\infty} \frac{\Phi_n(\sigma)}{d_\omega(n)} = (\sigma - \hat{\sigma})^\omega \left[1 + \sum_{i=\omega+1}^{k} \hat{d}_i(\sigma - \hat{\sigma})^{i-\omega}\right], \tag{A.21}$$

which follows from Eqs. (A.15) and (A.16).

For the proof of parts (2) and (3) we start by rewriting $\Phi_n(\hat{\sigma}_l(n)) = 0$ in the form

$$-(\hat{\sigma}_l(n) - \hat{\sigma})^\omega = \frac{\sum_{i=0}^{\omega-1}[d_i(n)/d_\omega(n)](\hat{\sigma}_l(n) - \hat{\sigma})^i}{1 + \sum_{i=\omega+1}^{k}[d_i(n)/d_\omega(n)](\hat{\sigma}_l(n) - \hat{\sigma})^{i-\omega}}. \tag{A.22}$$

Now by the assumptions in Eq. (A.16) and the fact that $\hat{\sigma}_l(n) - \hat{\sigma} = \mathrm{o}(1)$ as $n \to \infty$, which follows from part (1), the denominator of Eq. (A.22) is asymptotically equal to 1 as $n \to \infty$.

If $\omega = 1$, the numerator of Eq. (A.22) is simply $d_0(n)/d_\omega(n)$, so that we immediately have Eq. (A.17).

For arbitrary $\omega \geqslant 1$ we start by letting $\hat{\sigma}_l(n) - \hat{\sigma} = \epsilon_1^n \chi_l(n)$. Then Eq. (A.22) can be written in the form

$$\sum_{j=0}^{\omega-1} c_{lj}(n)[\chi_l(n)]^j + [\chi_l(n)]^\omega = 0, \tag{A.23}$$

where

$$c_{lj}(n) = \frac{[d_j(n)/d_\omega(n)]\epsilon_1^{(j-\omega)n}}{1 + \sum_{i=\omega+1}^{k}[d_i(n)/d_\omega(n)](\hat{\sigma}_l(n) - \hat{\sigma})^{i-\omega}}, \quad 0 \leqslant j \leqslant \omega - 1. \tag{A.24}$$

Substituting Eqs. (A.18) and (A.19) in Eq. (A.24), and recalling that the denominator in Eq. (A.24) is asymptotically equal to 1 as $n \to \infty$, we see that

$$c_{lj}(n) = \mathrm{O}\left(\prod_{r=1}^{\omega-j}\left(\frac{\epsilon_r}{\epsilon_1}\right)^n\right) = \mathrm{O}(1) \quad \text{as } n \to \infty,\ 0 \leqslant j \leqslant \omega - 1. \tag{A.25}$$

Now $\chi_l(n)$ is a zero of the *fixed* monic polynomial $P(\lambda) = \sum_{j=0}^{\omega-1} c_{lj}(n)\lambda^j + \lambda^\omega$, and all the zeros of this polynomial are bounded in modulus by $\max(1, \sum_{j=0}^{\omega-1} |c_{lj}(n)|)$, which is itself bounded as $n \to \infty$ by Eq. (A.25). Hence $|\chi_l(n)|$ is bounded as $n \to \infty$. This proves Eq. (A.20). □

We now go back to the zeros of $H_n(\sigma)$.

Lemma A.5. *Assume that the conditions of Lemma* A.3 *hold, and denote the zeros of* $H_n(\sigma)$ *that tend to* $\sigma_1, \ldots, \sigma_k$ *by* $\sigma_1(n), \ldots, \sigma_k(n)$, *respectively. For* $s = 1, 2, \ldots, k$, *we have*

$$\sigma_s(n) = \sigma_s + \mathrm{O}\left(\left|\frac{\zeta_{k+1}}{\zeta_s}\right|^n\right) \quad \text{as } n \to \infty. \tag{A.26}$$

When σ_s *is simple, i.e.,* $\sigma_s \neq \sigma_j$ *for* $s \neq j$, *Eq.* (A.26) *can be refined optimally in the following way: Let* r *be that positive integer for which*

$$|\zeta_k| > |\zeta_{k+1}| = \cdots = |\zeta_{k+r}| > |\zeta_{k+r+1}| \tag{A.27}$$

and denote

$$W_{1,2,\ldots,s-1,s+1,\ldots,k,k+i} = W_{[s;k+i]}. \tag{A.28}$$

Then

$$\sigma_s(n) \sim \sigma_s - \sum_{i=1}^{r} \frac{W_{[s;k+i]}}{W_{1,2,\ldots,k}} (\sigma_s - \sigma_{k+i}) \left(\frac{\zeta_{k+i}}{\zeta_s}\right)^n \quad \text{as } n \to \infty. \tag{A.29}$$

Proof. We start by writing

$$H_n(\sigma) = \sum_{i=0}^{k} \frac{1}{i!} H_n^{(i)}(\sigma_s)(\sigma - \sigma_s)^i. \tag{A.30}$$

In light of Lemma A.4 we now need to analyze the $H_n^{(i)}(\sigma_s)$.

Assume that σ_s is simple. Then, letting $\sigma = \sigma_s$ in Eq. (A.9), we have

$$H_n(\sigma_s) \sim \sum_{\substack{j_1 < j_2 < \cdots < j_k \\ j_p \neq s,\ 1 \leqslant p \leqslant k}} W_{j_1, j_2, \ldots, j_k} \left[\prod_{p=1}^{k} (\sigma_s - \sigma_{j_p})\right] \left(\prod_{p=1}^{k} \zeta_{j_p}^n\right) \tag{A.31}$$

as all the terms in the summation having $j_p = s$ for any one of the j_p, $1 \leqslant p \leqslant k$, vanish. By Eqs. (A.12) and (A.27) and the assumption that σ_s is simple, the dominant part of the summation on the right-hand side of Eq. (A.31) is seen to be the sum of those terms having the indices

$$j_1, j_2, \ldots, j_k = 1, 2, \ldots, s-1, s+1, \ldots, k, k+i, \quad 1 \leqslant i \leqslant r,$$

so that

$$H_n(\sigma_s) \sim \left\{ \sum_{i=1}^{r} W_{[s;k+i]} \left[\prod_{\substack{j=1 \\ j\neq s}}^{k} (\sigma_s - \sigma_j) \right] (\sigma_s - \sigma_{k+i}) \left(\frac{\zeta_{k+i}}{\zeta_s} \right)^n \right\} \left(\prod_{j=1}^{k} \zeta_j^n \right). \quad \text{(A.32)}$$

Now by Eq. (A.14) and by the assumption that σ_s is simple

$$H_n'(\sigma_s) = \frac{\mathrm{d}}{\mathrm{d}\sigma} H_n(\sigma)\big|_{\sigma=\sigma_s} \sim W_{1,2,\ldots,k} \left[\prod_{\substack{j=1 \\ j\neq s}}^{k} (\sigma_s - \sigma_j) \right] \left(\prod_{j=1}^{k} \zeta_j^n \right) \neq 0. \quad \text{(A.33)}$$

Similarly, $H_n^{(i)}(\sigma_s)$ for $i \geqslant 2$ are of the same order as $H_n'(\sigma_s)$. Therefore, part (2) of Lemma A.4 applies with $d_i(n) = H_n^{(i)}(\sigma_s)/i!$, $\omega = 1$, $\epsilon_1 = |\zeta_{k+1}/\zeta_s|$, and $\hat{\sigma} = \sigma_s$, and we have

$$\sigma_s(n) - \sigma_s \sim -\frac{H_n(\sigma_s)}{H_n'(\sigma_s)}, \quad \text{(A.34)}$$

which, upon invoking Eqs. (A.32) and (A.33), produces the result in Eq. (A.29) and also that in Eq. (A.26).

If σ_s has multiplicity $\omega > 1$, i.e., if $\sigma_s = \sigma_{s+1} = \cdots = \sigma_{s+\omega-1}$, then the analysis of the $H_n^{(i)}(\sigma_s)$ becomes more involved. First, for $i \geqslant \omega$ the dominant term of $H_n(\sigma)$ is obtained by differentiating the term with $j_1, \ldots, j_k = 1, \ldots, k$, and setting $\sigma = \sigma_s$ in it, and is of order $|\zeta_1 \cdots \zeta_k|^n$ as $n \to \infty$. In particular,

$$H_n^{(\omega)}(\sigma_s)/\omega! \sim W_{1,2,\ldots,k} \left(\prod_{j=1}^{k} \zeta_j^n \right) \left[\prod_{\substack{j=1 \\ \sigma_j \neq \sigma_s}}^{k} (\sigma_s - \sigma_j) \right] \neq 0. \quad \text{(A.35)}$$

For $i = 0$ set $\sigma = \sigma_s$ in Eq. (A.9). We see that all the terms having any one of their indices $j_1, \ldots, j_k$ equal to $s, s+1, \ldots, s+\omega-1$ vanish. Therefore,

$$H_n(\sigma_s) = \mathrm{O}\left(\left(\prod_{j=1}^{k} \zeta_j^n \right) \left(\prod_{l=1}^{\omega} \left| \frac{\zeta_{k+l}}{\zeta_s} \right|^n \right) \right) \quad \text{as } n \to \infty. \quad \text{(A.36)}$$

For $i = 1$ differentiate Eq. (A.9) term by term and set $\sigma = \sigma_s$ there. Now all the terms having any two of their indices $j_1, \ldots, j_k$ equal to $s, s+1, \ldots, s+\omega-1$ vanish. Therefore,

$$H_n'(\sigma_s) = \mathrm{O}\left(\left(\prod_{j=1}^{k} \zeta_j^n \right) \left(\prod_{l=1}^{\omega-1} \left| \frac{\zeta_{k+l}}{\zeta_s} \right|^n \right) \right) \quad \text{as } n \to \infty. \quad \text{(A.37)}$$

For $i \leqslant \omega - 1$ differentiate Eq. (A.9) i times term by term and set $\sigma = \sigma_s$ there. All the terms having any $i+1$ of their indices $j_1, \ldots, j_k$ equal to $s, s+1, \ldots, s+\omega-1$ vanish. Therefore, for $0 \leqslant i \leqslant \omega$,

$$H_n^{(i)}(\sigma_s) = \mathrm{O}\left(\left(\prod_{j=1}^{k}\zeta_j^n\right)\left(\prod_{l=1}^{\omega-i}\left|\frac{\zeta_{k+l}}{\zeta_s}\right|^n\right)\right) \quad \text{as } n \to \infty. \tag{A.38}$$

Hence part (3) of the previous lemma applies with $d_i(n) = H_n^{(i)}(\sigma_s)/i!$, $\epsilon_i = |\zeta_{k+i}/\zeta_s|$, and $\hat{\sigma} = \sigma_s$, and we obtain Eq. (A.26). (The reader is urged to verify Eqs. (A.36)–(A.38) for small values of k and ω.)

This completes the proof. □

A.3. A further result for simple σ_s when $|\zeta_k| > |\zeta_{k+l}|$

Lemma A.6. *Assume that the conditions of Lemma* A.3 *hold, and denote the zeros of $H_n(\sigma)$ that tend to $\sigma_1, \ldots, \sigma_k$ by $\sigma_1(n), \ldots, \sigma_k(n)$, respectively. Let σ_s be simple for some $s \in \{1, \ldots, k\}$. Then the solution of the homogeneous system of equations, cf. Eq.* (A.5),

$$\sum_{i=1}^{k} u_{ri}^{(n)}(\sigma_s(n))\xi_{si}(n) = 0, \quad 1 \leqslant r \leqslant k \tag{A.39}$$

for n sufficiently large, is unique up to a multiplicative constant, and satisfies

$$\sum_{i=1}^{k}\alpha_{iq}\xi_{si}(n) = \begin{cases} \mathrm{O}(1) & \text{at most, } q \geqslant k+1, \\ 1+\mathrm{o}(1) & \text{precisely, } q = s, \\ \mathrm{O}(\zeta_{k+1}^n\zeta_q^{-n}) & \text{at most, } 1 \leqslant q \leqslant k,\ q \neq s, \text{ as } n \to \infty, \end{cases} \tag{A.40}$$

when scaled appropriately.

Proof. First, the matrix of the system in Eq. (A.39) is singular as its determinant is simply $H_n(\sigma_s(n))$, which itself is zero. By the assumption that σ_s is simple, we see from Lemma A.5 that $\sigma_s(n) \neq \sigma_j(n)$ for $j \neq s$ for all large n. Thus the matrix of the system in Eq. (A.39) has rank $k-1$ exactly. This implies that the solution of Eq. (A.39) is unique up to a multiplicative constant, and that it can be obtained from $k-1$ of the equations there.

Next, Eq. (A.13) implies that $Z_{1,\ldots,k}(\alpha) \neq 0$ and $Z_{1,\ldots,k}(\beta) \neq 0$ simultaneously. Now $Z_{1,\ldots,k}(\beta) \neq 0$ guarantees that for any $s, 1 \leqslant s \leqslant k$, there exists a $(k-1) \times (k-1)$ minor of the determinant representation of $Z_{1,\ldots,k}(\beta)$, cf. Eq. (A.7), that does not include the sth row and does not vanish. Without loss of generality and for simplicity of notation, we assume that this minor is obtained by deleting the sth row and the kth column. This amounts to

$$Z_{1,2,\ldots,s-1,s+1,\ldots,k}(\beta) \neq 0. \tag{A.41}$$

With this we now assume, without loss of generality, that the $k-1$ equations mentioned at the end of the previous paragraph are the first $k-1$ equations of Eq. (A.39). In view of this, it is easy to verify by Cramer's rule that for any scalars $\delta_1, \delta_2, \ldots, \delta_k$, we have

$$\sum_{i=1}^{k} \delta_i \xi_{si}(n) = \begin{vmatrix} \delta_1 & \delta_2 & \cdots & \delta_k \\ u_{11} & u_{12} & \cdots & u_{1k} \\ u_{21} & u_{22} & \cdots & u_{2k} \\ \vdots & \vdots & & \vdots \\ u_{k'1} & u_{k'2} & \cdots & u_{k'k} \end{vmatrix} \quad \text{with } k' = k-1, \tag{A.42}$$

where we have denoted $u_{pq} \equiv u_{pq}^{(n)}(\sigma_s(n))$ and we have normalized $\xi_{sl}(n)$ appropriately. Substituting now $\delta_i = \alpha_{iq}$ and Eq. (A.6) in Eq. (A.42), and proceeding exactly as in the proof of Lemma A.3, we obtain

$$\sum_{i=1}^{k} \alpha_{iq} \xi_{si}(n) \sim \sum_{j_1<j_2<\cdots<j_{k'}} Z_{j_1,\ldots,j_{k'}}(\beta) Z_{q,j_1,\ldots,j_{k'}}(\alpha) \left[\prod_{p=1}^{k'} (\sigma_s(n) - \sigma_{j_p})\right] \left(\prod_{p=1}^{k'} \zeta_{j_p}^n\right). \tag{A.43}$$

Obviously, all those terms in Eq. (A.43) for which any one of the indices $j_1, \ldots, j_{k'}$ takes on the value q vanish on account of $Z_{q,j_1,\ldots,j_{k'}}(\alpha)$ vanishing. That is to say, the indices $j_1, \ldots, j_{k'}$ in Eq. (A.43) take on all values except q.

Let us now analyze Eq. (A.43) for all values of q. First, for $q=s$ the dominant term there has the indices

$$j_1, j_2, \ldots, j_{k'} = 1, 2, \ldots, s-1, s+1, \ldots, k$$

and, by Lemma A.5, as $n \to \infty$, is asymptotically equal to

$$(-1)^{s-1} Z_{1,\ldots,s-1,s+1,\ldots,k}(\beta) Z_{1,2,\ldots,k}(\alpha) \left[\prod_{\substack{j=1 \\ j\neq s}}^{k} (\sigma_s - \sigma_j)\right] \left(\prod_{\substack{j=1 \\ j\neq s}}^{k} \zeta_j^n\right).$$

The important point here is that this term is precisely $O(\pi^n)$ as $n \to \infty$, where $\pi \equiv (\prod_{j=1}^{k} \zeta_j)/\zeta_s$, since the constant factors in it are all nonzero by Eqs. (A.13) and (A.41). Next, for $1 \leqslant q \leqslant k$, $q \neq s$, we see that the dominant terms have indices $j_1, \ldots, j_{k'}$, that take on the values $1, 2, \ldots, q-1, q+1, \ldots, k$ including s, or the values $1, 2, \ldots, k, k+i$ excluding q and $s, i = 1, 2, \ldots, r$. Invoking also Lemma A.5, we see that all these terms are at most $O(\pi^n \zeta_{k+1}^n / \zeta_q^n)$ as $n \to \infty$. Finally, for $q \geqslant k+1$ the dominant term has the same indices as in the case of $q=s$ and is $O(\pi^n)$ as $n \to \infty$. This completes the proof. □

A.4. Treatment of $H_n(\sigma)$ and its zeros for $|\zeta_k| = |\zeta_{k+l}|$

The results in Lemmas A.3, A.5, and A.6 are made possible especially by the condition $|\zeta_k| > |\zeta_{k+1}|$ in Eq. (A.12). If this condition is not satisfied, then the proofs of these results are not valid, and the question arises as to whether they can be saved or modified in a simple manner. Lemmas A.7 and A.8 give a detailed treatment of this question regarding Lemma A.3 for $H_n(\sigma)$ and Lemma A.5 for the σ_s, respectively. We shall not pursue the modification of Lemma A.6.

Lemma A.7. *In Lemma* A.2 *let*

$$|\zeta_1| \geqslant \cdots \geqslant |\zeta_t| > |\zeta_{t+1}| = \cdots = |\zeta_{t+r}| > |\zeta_{t+r+1}| \geqslant \cdots \tag{A.44}$$

for some $t \geqslant 1$ and $r \geqslant 2$, and let

$$t+1 \leqslant k < t+r. \tag{A.45}$$

1. *When $\zeta_{t+1}, \ldots, \zeta_{t+r}$ are not all the same, assume that*

$$R(n;\sigma) = \sum_{t+1 \leqslant j_{t+1} < \cdots < j_k \leqslant t+r} W_{1,2,\ldots,t,j_{t+1},\ldots,j_k} \left[\prod_{p=t+1}^{k} (\sigma - \sigma_{j_p})\right] \left(\prod_{p=t+1}^{k} \frac{\zeta_{j_p}}{|\zeta_{j_p}|}\right)^n \not\equiv 0 \tag{A.46}$$

for some integer n. Then there exist integers $0 \leqslant n_0 < n_1 < n_2 < \cdots$, for which $\{R(n_i;\sigma)\}_{i=0}^{\infty}$ has a limit. Also, with appropriate constants d_n, the subsequence $\{d_{n_i} H_{n_i}(\sigma)\}_{i=0}^{\infty}$ converges to a polynomial in σ of degree $t+q \leqslant k$, whose zeros are $\sigma_1, \sigma_2, \ldots, \sigma_t$ and $\sigma'_1, \ldots, \sigma'_q$, the latter being the zeros of the limit of the subsequence of polynomials $\{R(n_i;\sigma)\}_{i=0}^{\infty}$. Actually, for this subsequence

$$d_n H_n(\sigma) = \left[\prod_{j=1}^{t} (\sigma - \sigma_j)\right] \left[\prod_{j=1}^{q} (\sigma - \sigma'_j)\right] + \mathrm{O}(\eta_t^n) \quad \text{as } n \to \infty \tag{A.47}$$

with

$$\eta_t = \max\left(\left|\frac{\zeta_{t+1}}{\zeta_t}\right|, \left|\frac{\zeta_{t+r+1}}{\zeta_{t+r}}\right|\right). \tag{A.48}$$

2. *When $\zeta_{t+1} = \cdots = \zeta_{t+r}$, assume that*

$$T(\sigma) = \sum_{t+1 \leqslant j_{t+1} < \cdots < j_k \leqslant t+r} W_{1,2,\ldots,t,j_{t+1},\ldots,j_k} \left[\prod_{p=t+1}^{k} (\sigma - \sigma_{j_p})\right] \not\equiv 0. \tag{A.49}$$

Then, with the proper normalization constants d_n, the sequence $\{d_n H_n(\sigma)\}_{n=0}^{\infty}$ converges to a polynomial in σ of degree $t+q \leqslant k$ whose zeros are $\sigma_1, \sigma_2, \ldots, \sigma_t$ and $\sigma'_1, \ldots, \sigma'_q$, the latter being the zeros of the polynomial $T(\sigma)$. If $\sum_{t+1 \leqslant j_{t+1} < \cdots < j_k \leqslant t+r} W_{1,2,\ldots,t,j_{t+1},\ldots,j_k} \neq 0$, then $t+q = k$ exactly. This time the whole sequence $\{d_n H_n(\sigma)\}_{n=0}^{\infty}$ satisfies Eqs. (A.47) *and* (A.48).

Proof. The proof can be accomplished as that of Lemma 2.4 in [20]. We leave the details to the reader. □

Lemma A.8. *Assume the conditions of Lemma* A.7, *and let* $s \in \{1, 2, \ldots, t\}$. *Then*

$$\sigma_s(n) = \sigma_s + \mathrm{O}\left(\left|\frac{\zeta_{t+1}}{\zeta_s}\right|^n\right) \quad \text{as } n \to \infty \tag{A.50}$$

when $\zeta_{t+1} = \cdots = \zeta_{t+r}$. *When* $\zeta_{t+1}, \ldots, \zeta_{t+r}$ *are not all the same, Eq.* (A.50) *holds with n replaced by* n_i, *where* $\{d_{n_i} H_{n_i}(\sigma)\}_{i=0}^{\infty}$ *is the convergent subsequence of part* (1) *of Lemma* A.7.

Proof. The proof is almost identical to that of Lemma A.5. We shall mention the important points for the case in which $\zeta_{t+1}, \ldots, \zeta_{t+r}$ are not all the same. First, for arbitrary $\sigma \notin \{\sigma_1, \ldots, \sigma_t, \sigma'_1, \ldots, \sigma'_q\}$, we have

$$H_{n_i}(\sigma) \sim \left[\prod_{j=1}^{t}(\sigma - \sigma_j)\right] R(n_i; \sigma) \left(\prod_{j=1}^{t} \zeta_j^{n_i}\right) |\zeta_{t+1}|^{n_i(k-t)}. \tag{A.51}$$

Next, if σ_s is of multiplicity ω in $\{\sigma_1, \ldots, \sigma_t\}$ and $\sigma_s \notin \{\sigma'_1, \ldots, \sigma'_q\}$, then from Eq. (A.51) we have

$$H_{n_i}^{(\omega)}(\sigma_s)/\omega! \sim \left[\prod_{\substack{j=1 \\ \sigma_j \neq \sigma_s}}^{t} (\sigma_s - \sigma_j)\right] R(n_i; \sigma_s) \left(\prod_{j=1}^{t} \zeta_j^{n_i}\right) |\zeta_{t+1}|^{n_i(k-t)} \neq 0, \tag{A.52}$$

since $\lim_{i\to\infty} R(n_i; \sigma_s)$ is defined and nonzero. Also,

$$H_{n_i}^{(m)}(\sigma_s) = \mathrm{O}\left(\left(\prod_{j=1}^{t} \zeta_j^{n_i}\right) |\zeta_{t+1}|^{n_i(k-t)}\right) \quad \text{as } i \to \infty, \ \omega + 1 \leqslant m \leqslant k. \tag{A.53}$$

(Both Eqs. (A.52) and (A.53) are obtained by differentiating Eq. (A.51).) Finally,

$$H_{n_i}^{(m)}(\sigma_s) = \mathrm{O}\left(\left(\prod_{j=1}^{k} \zeta_j^{n_i}\right) \prod_{l=1}^{\omega-m} \left|\frac{\zeta_{k+l}}{\zeta_s}\right|^{n_i}\right) \quad \text{as } i \to \infty, \ 0 \leqslant m \leqslant \omega - 1. \tag{A.54}$$

Now proceed as in the proof of Lemma A.5 to get to Eq. (A.50) with n there replaced by n_i, recalling also the fact that $|\zeta_k| = |\zeta_{k+1}| = |\zeta_{t+1}|$.

The proof of the case in which $\zeta_{t+1} = \cdots = \zeta_{t+r}$ is completely analogous and slightly easier, and is left to the reader. □

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