SIAM J. MATRIX ANAL. APPL.
Vol. 16, No. 4, pp. 1341–1369, October 1995

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APPLICATION OF VECTOR-VALUED RATIONAL APPROXIMATIONS TO THE MATRIX EIGENVALUE PROBLEM AND CONNECTIONS WITH KRYLOV SUBSPACE METHODS *

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Abstract. Let $F(z)$ be a vector-valued function $F : \mathbf{C} \to \mathbf{C}^N$, which is analytic at $z = 0$ and meromorphic in a neighborhood of $z = 0$, and let its Maclaurin series be given. In a recent work [*J. Approx. Theory*, 76 (1994), pp. 89–111] by the author, vector-valued rational approximation procedures for $F(z)$ that are based on its Maclaurin series, were developed, and some of their convergence properties were analyzed in detail. In particular, a Koenig-type theorem concerning their poles and a de Montessus-type theorem concerning their uniform convergence in the complex plane were given. With the help of these theorems it was shown how optimal approximations to the poles of $F(z)$ and the principal parts of the corresponding Laurent series expansions can be obtained. In this work we use these rational approximation procedures in conjunction with power iterations to develop bona fide generalizations of the power method for an arbitrary $N \times N$ matrix that may or may not be diagonalizable. These generalizations can be used to obtain simultaneously several of the largest distinct eigenvalues and corresponding eigenvectors and other vectors in the invariant subspaces. We provide interesting constructions for both nondefective and defective eigenvalues and the corresponding invariant subspaces, and present a detailed convergence theory for them. This is made possible by the observation that vectors obtained by power iterations with a matrix are actually coefficients of the Maclaurin series of a vector-valued rational function, whose poles are the reciprocals of some or all of the nonzero eigenvalues of the matrix being considered, while the coefficients in the principal parts of the Laurent expansions of this rational function are vectors in the corresponding invariant subspaces. In addition, it is shown that the generalized power methods of this work are equivalent to some Krylov subspace methods, among them the methods of Arnoldi and Lanczos. Thus, the theory of the present work provides a set of completely new results and constructions for these Krylov subspace methods. At the same time this theory suggests a new mode of usage for these Krylov subspace methods that has been observed to possess computational advantages over their common mode of usage in some cases. We illustrate some of the theory and conclusions derived from it with numerical examples.

Key words. Krylov subspace methods, method of Arnoldi, method of Lanczos, power iterations, generalized power methods, diagonalizable matrices, defective matrices, eigenvalues, invariant subspaces, vector-valued rational approximations

AMS subject classifications. 30E10, 41A20, 65F15, 65F30, 65F50

1. Introduction.

Let $F(z)$ be a vector-valued function, $F : \mathbf{C} \to \mathbf{C}^N$, which is analytic at $z = 0$ and meromorphic in a neighborhood of $z = 0$, and let its Maclaurin series be given as

$$F(z) = \sum_{m=0}^{\infty} u_m z^m, \tag{1.1}$$

where u_m are fixed vectors in $\mathbf{C}^N$.

*Received by the editors December 31, 1992; accepted for publication (in revised form) by A. Berman September 1, 1994. The results of this paper were presented at the International Meeting on Approximation, Interpolation, and Summability, Tel-Aviv, June 1990, the International Congress on Extrapolation and Rational Approximation, Tenerife, January 1992, and the Lanczos International Centenary Conference, Raleigh, North Carolina, December 1993.

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In a recent work by the author [Si6] three types of vector-valued rational approximation procedures, entirely based on the expansion in (1.1), were proposed. For each of these procedures the rational approximations have two indices, n and k, attached to them, and thus form a two-dimensional table akin to the Padé table or the Walsh array. Let us denote the (n,k) entry of this table by $F_{n,k}(z)$. Then $F_{n,k}(z)$, if it exists, is defined to be of the form

$$F_{n,k}(z)=\frac{\sum_{j=0}^{k}c_j^{(n,k)}z^{k-j}F_{n+\nu+j}(z)}{\sum_{j=0}^{k}c_j^{(n,k)}z^{k-j}}\equiv\frac{P_{n,k}(z)}{Q_{n,k}(z)}\ \text{with}\ c_k^{(n,k)}=Q_{n,k}(0)=1, \tag{1.2}$$

where ν is an arbitrary but otherwise fixed integer ≥ -1, and

$$F_m(z)=\sum_{i=0}^{m}u_iz^i,\ m=0,1,2,\ldots;\qquad F_m(z)\equiv 0\quad\text{for } m<0, \tag{1.3}$$

and the $c_j^{(n,k)}$ are scalars that depend on the approximation procedure being used.

If we denote the three approximation procedures by SMPE, SMMPE, and STEA, then the $c_j^{(n,k)}\equiv c_j$ for each of the three procedures, are defined such that they satisfy a linear system of equations of the form

$$\sum_{j=0}^{k-1}u_{ij}c_j=-u_{ik},\quad 0\leq i\leq k-1;\qquad c_k=1, \tag{1.4}$$

where u_{ij} are scalars defined as

$$u_{ij}=\begin{cases}(u_{n+i},u_{n+j}) & \text{for SMPE,}\\ (q_{i+1},u_{n+j}) & \text{for SMMPE,}\\ (q,u_{n+i+j}) & \text{for STEA.}\end{cases} \tag{1.5}$$

Here $(\cdot,\cdot)$ is an inner product--not necessarily the standard Euclidean inner product—whose homogeneity property is such that $(\alpha x,\beta y)=\bar{\alpha}\beta(x,y)$ for x,y in $\mathbf{C}^N$ and α,β in $\mathbf{C}$. The vectors $q_1,q_2,\ldots,$ form a linearly independent set, and the vector q is nonzero. Obviously, $F_{n,k}(z)$ exists if the linear system in (1.4) has a solution for $c_0,c_1,\ldots,c_{k-1}$.

It is easy to verify that for SMPE the equations in (1.4) involving $c_0,c_1,\ldots,c_{k-1}$ are the normal equations for the least squares problem

$$\min_{c_0,c_1,\ldots,c_{k-1}}\left\|\sum_{j=0}^{k-1}c_ju_{n+j}+u_{n+k}\right\|, \tag{1.6}$$

where the norm $\|\cdot\|$ is that induced by the inner product $(\cdot,\cdot)$, namely, $\|x\|=\sqrt{(x,x)}$.

As is clear from (1.2) and (1.3), the numerator of $F_{n,k}(z)$ is a vector-valued polynomial of degree at most $n+\nu+k$, whereas its denominator is a scalar polynomial of degree at most k.

As can be seen from (1.4) and (1.5), the denominator polynomial $Q_{n,k}(z)$ is constructed from $u_n,u_{n+1},\ldots,u_{n+k}$ for SMPE and SMMPE, and from $u_n,u_{n+1},\ldots,u_{n+2k-1}$ for STEA. Once the denominators have been determined, the numerators involve $u_0,u_1,\ldots,u_{n+\nu+k}$ for all three approximation procedures.

The approximation procedures above are very closely related to some vector extrapolation methods. In fact, as is stated in Theorem 2.3 in Section 2 of [Si6], $F_{n,k}(z)$ for SMPE, SMMPE, and STEA are obtained by applying some generalized versions of the minimal polynomial extrapolation (MPE), the modified minimal polynomial extrapolation (MMPE), and the topological epsilon algorithm (TEA), respectively, to the vector sequence $F_m(z), m = 0, 1, 2, \ldots$. For early references pertaining to these methods and their description, see the survey paper of Smith, Ford, and Sidi [SmFSi], and for recent developments pertaining to their convergence, stability, implementation, and other additional properties, see the papers by Sidi [Si1], [Si2], [Si5], Sidi and Bridger [SiB], Sidi, Ford, and Smith [SiFSm], and Ford and Sidi [FSi]. The above mentioned generalizations of vector extrapolation methods are given in [SiB, (1.16) and (1.17)].

A detailed convergence analysis for the approximations $F_{n,k}(z)$ as $n \to \infty$ was given in [Si6], whose main results can be verbally summarized as follows: (i) Under certain conditions the denominators $Q_{n,k}(z)$ converge, and their zeros, k in number, tend to the k poles of $F(z)$ that are closest to the origin. This is a Koenig-type result and is proved in Theorems 4.1 and 4.5 of [Si6], where the precise rates of convergence are also given for both simple and multiple poles of $F(z)$, and optimal approximations to multiple poles are constructed in a simple way. (ii) Under the same conditions $F_{n,k}(z)$ converges to $F(z)$ uniformly in any compact subset of the circle containing the above-mentioned k poles of $F(z)$ with these poles excluded. This is a de Montessus-type result and is proved in Theorem 4.2 of [Si6]. (iii) The principal parts of the Laurent expansions of $F(z)$ about its poles, simple or multiple, can be constructed from $F_{n,k}(z)$ only. This construction, along with its convergence theory, is provided in Theorem 4.3 of [Si6].

It turns out that the denominator polynomials $Q_{n,k}(z)$ are very closely related to some recent extensions of the power method for the matrix eigenvalue problem, see [SiB, §6] and [Si3]. Specifically, if the vectors u_m of (1.1) are obtained from $u_m = Au_{m-1}, m = 1, 2, \ldots$, with u_0 arbitrary, and A being a complex $N \times N$ and, in general, nondiagonalizable matrix, then the reciprocals of the zeros of the polynomial $Q_{n,k}(z)$ are approximations to the k largest distinct and, in general, defective eigenvalues of A, counted according to their multiplicities, under certain conditions. In §3 of this work we provide precise error bounds for these approximations for $n \to \infty$ that are based on the results of Theorems 4.1 and 4.5 of [Si6]. While the approximations to nondefective eigenvalues have optimal accuracy in some sense, those that correspond to defective eigenvalues do not. In this paper we also show how approximations of optimal accuracy to defective eigenvalues can be constructed solely from $Q_{n,k}(z)$, providing their convergence theory for $n \to \infty$ at the same time. We then extend the treatment of [SiB] and [Si3] to cover the corresponding invariant subspaces in general, and the corresponding eigenvectors in particular. For example, we actually show how the eigenvectors corresponding to the largest distinct eigenvalues, whether these are defective or not, can be approximated solely in terms of the vectors u_j, and provide precise rates of convergence for them. The key to these results is the observation that the vector-valued power series $\sum_{m=0}^{\infty} u_m z^m$ actually represents a vector-valued *rational* function $F(z)$ whose poles are the reciprocals of some or all of the nonzero eigenvalues of A, depending on the spectral decomposition of u_0, and that corresponding eigenvectors (and certain combinations of eigenvectors and principal vectors) are related to corresponding principal parts of the Laurent expansions of the function $F(z)$. The main results of §3 pertaining to eigenvalues are given in Theorem 3.1, while those pertaining to eigenvectors and invariant subspaces are given in Theorem 3.2

and the subsequent paragraphs. A detailed description of the properties of the power iterations $u_m = Au_{m-1}, m = 1, 2, \ldots$, is provided in §2.

In §4 we present a short review of general projection methods and Krylov subspace methods for the matrix eigenvalue problem. Of particular interest to us are the methods of Arnoldi [A] and Lanczos [L], which are described in this section.

In §5 we show that the extensions of the power method developed and analyzed in §3 are very closely related to Krylov subspace methods. In particular, we show that the reciprocals of the k poles and the corresponding residues of the rational approximations $F_{n,k}(z)$ (with $\nu = -1$) obtained from the SMPE, SMMPE, and STEA procedures are the Ritz values and the Ritz vectors, respectively, of certain Krylov subspace methods of order k for the matrix A starting with the power iteration u_n. Specifically, the methods of Arnoldi and Lanczos are related to the $F_{n,k}(z)$ obtained from the SMPE and STEA procedures, respectively, precisely in this sense when $(\cdot, \cdot)$ in (1.5) is the standard Euclidean inner product. The main results of §5 concerning this are summarized in Theorem 5.4 and Corollary 5.5. In addition, Theorem 5.6 gives some optimality properties of the Arnoldi method.

Now the Ritz values and Ritz vectors obtained from Krylov subspace methods are normally used as approximations to nondefective eigenpairs. They are not very effective for defective eigenpairs. Since we know that the generalized power methods based on the SMPE, SMMPE, and STEA procedures are related to Krylov subspace methods, the constructions for approximating defective eigenvalues and their corresponding invariant subspaces that originate from generalized power methods and that are given in §3 are entirely new as far as Krylov subspace methods are concerned. Similarly, all of the convergence results of §3, whether they pertain to defective or nondefective eigenvalues and their corresponding invariant subspaces, are new and totally different from the known analyses provided by Kaniel [K], Paige [Pai], and Saad [Sa1], [Sa2]. Some of these analyses can also be found in Parlett [Par2] and Golub and Van Loan [GV]. The last two references also give a very thorough treatment of the computational aspects of Krylov subspace methods.

In §6 we show how the Ritz values and Ritz vectors obtained in a stable way from the common implementations of the Arnoldi and Lanczos methods can be used in constructing the approximations to the defective eigenvalues and their corresponding invariant subspaces in general and eigenvectors in particular.

In §7 we illustrate some of the theoretical results and claims of the paper with numerical examples.

In view of the connection between (1) the Krylov subspace methods and (2) the vector-valued rational approximations of [Si6] and the corresponding generalized power methods of the present work, we now summarize the main contributions of this paper.

(i) It is shown that Krylov subspace methods for the matrix eigenvalue problem are completely equivalent to methods founded on analytic function theory and rational approximations in the complex plane.

(ii) A mode of usage of Krylov subspace methods akin to the power method, in which one first iterates on an arbitrary initial vector many times and only then applies Krylov subspace methods, is proposed. This mode produces approximations only to the largest eigenvalues and their corresponding invariant subspaces.

(iii) The output from Krylov subspace methods, namely, the Ritz values and Ritz vectors, are used in constructing optimal approximations to defective eigenvalues and the corresponding eigenvectors and invariant subspaces. (The Ritz values and Ritz vectors by themselves are not good approximations to defective eigenvalues and

corresponding eivenvectors and invariant subspaces.)

(iv) A *complete* convergence theory for the generalized power methods is provided.

(v) This author's numerical experience suggests that at least in some cases the mode of usage proposed in this work and mentioned in (ii) above may produce the accuracy that is achieved by applying the Arnoldi method in the commonly known way using less storage and less computational work when the matrix being treated is large and sparse.

Before closing this section we note that the eigenvalue problem for defective matrices has received some attention in the literature. The problem of approximating the largest eigenvalue of a matrix when this eigenvalue is defective has been considered by Ostrowski [O], who proposes an extension of the Rayleigh quotient and inverse iteration and gives a thorough analysis for this extension. Parlett and Poole [ParPo] consider the properties of a wide range of projection methods within the framework of defective matrices. The convergence of the QR method for defective Hessenberg matrices has been analyzed in detail by Parlett [Par1]. The problem of determining the Jordan canonical form of defective matrices has been treated in Golub and Wilkinson [GW]. The use of power iterations in approximating defective eigenvalues is also treated to some extent in Wilkinson [W, Chap. 7] and Householder [H, Chap. 7].

Finally, we mention that the results of [Si6], as well as the application of vector-valued rational approximations to the matrix eigenvalue problem, were motivated by the developments in a recent work by the author [Si4] on the classical Padé approximants.

2. Properties of power iterations. Let A be an $N \times N$ matrix, which, in general, is complex and nondiagonalizable. Let u_0 be a given arbitrary vector in $\mathbf{C}^N$, and generate the vectors $u_1, u_2, \ldots$, according to

$$u_{j+1} = Au_j, \quad j \geq 0. \tag{2.1}$$

Denote by s the index of A, i.e., the size of the largest Jordan block of A with zero eigenvalue. Then u_m is of the form

$$u_m = \sum_{j=1}^{M} \left[\sum_{l=0}^{p_j} \tilde{a}_{jl} \binom{m}{l} \right] \lambda_j^m \quad \text{for } m \geq s, \tag{2.2}$$

where λ_j are some or all of the *distinct nonzero* eigenvalues of A, which we choose to order such that

$$|\lambda_1| \geq |\lambda_2| \geq |\lambda_3| \geq \cdots \geq |\lambda_M| > 0, \tag{2.3}$$

$p_j + 1 \equiv \omega_j$ are positive integers less than or equal to the dimension of the invariant subspace of A belonging to the eigenvalue λ_j, and $\tilde{a}_{jl}, 0 \leq l \leq p_j$, are linearly independent vectors in this invariant subspace. It turns out that the vector $\tilde{a}_{jp_j}$ is an *eigenvector* of A corresponding to λ_j, while the vectors $\tilde{a}_{ji}, i = 0, 1, \ldots, p_j - 1$, are combinations of eigenvectors *and* principal vectors of A corresponding to the eigenvalue λ_j. What is more, the subspaces

$$Y_i = \operatorname{span}\{\tilde{a}_{jl}, i \leq l \leq p_j\}, \qquad i = 0, 1, \ldots, p_j,$$

are invariant subspaces of A corresponding to the eigenvalue λ_j, and satisfy $Y_0 \supset Y_1 \supset \cdots \supset Y_{p_j}$.

Whether all distinct nonzero eigenvalues are present among $\lambda_1, \lambda_2, \ldots, \lambda_M$, the exact values of the ω_j, and the precise composition of the vectors $\tilde{a}_{jl}$, all depend on the spectral decomposition of the initial vector u_0. For a detailed derivation of the above see [SiB, §2].

Before we go on, we will only mention how to determine the maximum value that ω_j can assume. Suppose that the Jordan canonical form of A has several Jordan blocks whose eigenvalues are all equal to λ_j. Then the largest value that ω_j can assume is the size of the largest of these blocks. In general, for a randomly chosen vector u_0, ω_j will take on its maximum value. In cases where ω_j is theoretically less than this maximum value, rounding errors on a computer will ultimately force ω_j to take on its maximum value.

It is obvious from the above that

$$k_0 \equiv \sum_{j=1}^{M} (p_j + 1) = \sum_{j=1}^{M} \omega_j \leq N \tag{2.4}$$

and

$$\tilde{a}_{ji},\ 0 \leq i \leq p_j, 1 \leq j \leq M, \quad \text{are linearly independent.} \tag{2.5}$$

Also the minimal polynomial of the matrix A with respect to the vector u_s has degree $k_0 = \sum_{j=1}^{M} \omega_j$, i.e.,

$$k_0 = \min \left\{ k\colon \left(\sum_{i=0}^{k} \beta_i A^i \right) u_s = 0, \beta_k = 1 \right\}.$$

If defined as a monic polynomial, this polynomial is unique and divides the minimal polynomial of A, which, in turn, divides the characteristic polynomial of A. Furthermore, the minimal polynomial of A with respect to u_s is also the minimal polynomial of A with respect to u_m for all $m \geq s$. Consequently, any set of vectors $\{u_m, u_{m+1}, \ldots, u_{m+k}\}$ is linearly independent for $m \geq s$ provided $k < k_0$.

Now applying Lemma 3.1 of [Si6] in conjunction with (2.2), we conclude that the vector-valued power series $\sum_{m=0}^{\infty} u_m z^m$ represents the vector-valued *rational* function

$$F(z) = (I - zA)^{-1} u_0 = \sum_{j=1}^{M} \sum_{i=0}^{p_j} \frac{a_{ji}}{(1 - \lambda_j z)^{i+1}} + G(z), \tag{2.6}$$

in which the vectors a_{ji} are uniquely determined in terms of the $\tilde{a}_{jl}$ from

$$\tilde{a}_{jl} = \sum_{i=l}^{p_j} a_{ji} \binom{i}{i-l}, \quad 0 \leq l \leq p_j, \quad 1 \leq j \leq M, \tag{2.7}$$

and hence form a linearly independent set, and $G(z)$ is a vector-valued polynomial of degree at most $s - 1$. In fact, $G(z)$ is in the invariant subspace of A corresponding to the zero eigenvalue. Also, $a_{jp_j} = \tilde{a}_{jp_j}$, i.e., a_{jp_j} is an eigenvector of A corresponding to the eigenvalue λ_j, while for each $i, 0 \leq i \leq p_j - 1, a_{ji}$ is some other vector in the invariant subspace Y_i corresponding to the eigenvalue λ_j, and involves principal vectors as well as eigenvectors.

When the matrix A is diagonalizable, $p_j = 0$ for all j in (2.2) and hence in (2.6). If, in addition, A is normal, then its eigenvectors form an orthogonal set with respect to the standard Euclidean inner product, namely, $(x, y) = x^*y$, where x^* stands for the hermitian conjugate of x. Consequently, the vectors $\tilde{a}_{j0} = a_{j0}$ in (2.2) and (2.6) are orthogonal with respect to this inner product when A is normal.

Now that we have shown that the power series $\sum_{m=0}^{\infty} u_m z^m$ represents a rational function $F(z)$ that is analytic at $z = 0$ and has poles $z_j = \lambda_j^{-1}$ of respective multiplicities $\omega_j = p_j + 1, j = 1, 2, \ldots, M$, we can apply any one of the approximation procedures SMPE, SMMPE, or STEA to the power series $\sum_{m=0}^{\infty} u_m z^m$ to obtain the vector-valued rational approximations $F_{n,k}(z)$ to $F(z)$. We can then apply the theorems of §§4 and 5 of [Si6] to construct approximations to the eigenvalues λ_j and the vectors a_{ji} in (2.6) and (2.7).

It is important to note that the linear independence of the vectors a_{jl} is an important condition for the convergence of the SMPE and SMMPE procedures, but is not needed for the STEA procedure. In addition, we assume throughout that

$$\text{(2.8)} \qquad \begin{vmatrix} (q_1, a_{10}) & \cdots & (q_1, a_{1p_1}) & \cdots & (q_1, a_{t0}) & \cdots & (q_1, a_{tp_t}) \\ \vdots & & \vdots & & \vdots & & \vdots \\ (q_k, a_{10}) & \cdots & (q_k, a_{1p_1}) & \cdots & (q_k, a_{t0}) & \cdots & (q_k, a_{tp_t}) \end{vmatrix} \neq 0 \text{ for SMMPE,}$$

where $k = \sum_{j=1}^{t} w_j$, and that

$$\text{(2.9)} \qquad \prod_{j=1}^{t} (q, a_{jp_j}) \neq 0 \text{ for STEA.}$$

No additional assumption is needed for SMPE.

In order for (2.8) to hold it is necessary (but not sufficient) that the two sets of vectors $\{a_{ji} : 0 \leq i \leq p_j, 1 \leq j \leq t\}$ and $\{q_1, \ldots, q_k\}$, each be linearly independent, as has already been assumed.

3. Theoretical development of generalized power methods. In light of the developments of §2 and Theorems 4.1, 4.3, and 4.5 of [Si6] and the developments of §5 in the same paper, we approach the matrix eigenvalue problem as follows.

Given the vector u_0 that is picked arbitrarily, we generate the vectors $u_1, u_2, \ldots$, according to (2.1). We then fix the integers n and k, and determine the coefficients $c_j^{(n,k)}, j = 0, 1, \ldots, k$, of the denominator polynomial of $F_{n,k}(z)$ for one of the procedures SMPE, SMMPE, and STEA, by using $u_n, u_{n+1}, \ldots, u_{n+k}$ for SMPE and SMMPE, and $u_n, u_{n+1}, \ldots, u_{n+2k-1}$, for STEA. By Theorem 4.1 of [Si6] the zeros of the polynomial $\hat{Q}_{n,k}(\lambda) \equiv \lambda^{-k} Q_{n,k}(\lambda^{-1}) = \sum_{j=0}^{k} c_j^{(n,k)} \lambda^j$ are approximations to the k largest λ_j in (2.2), counted according to their multiplicities ω_j, provided the conditions stated in this theorem are satisfied. In case the matrix A is normal, the zeros of the polynomial $\hat{Q}_{n,k}(\lambda)$, obtained from SMPE and STEA with the standard Euclidean inner product, are even better approximations to the eigenvalues λ_j of A as follows from Theorem 4.5 of [Si6].

3.1. Treatment of eigenvalue approximations. Theorem 3.1 below, which is of constructive nature, summarizes all the relevant results concerning the approximations to the λ_j. The corresponding approximations to eigenvectors and other vectors in the invariant subspaces are subsequently obtained with the help of the developments

in §5 of [Si6], and the relevant results for this problem are summarized in Theorem 3.2 below.

We note that in this section we have adopted all of the notation of the previous sections.

THEOREM 3.1. *Let the matrix A and the vector sequence $u_m, m = 0, 1, 2, \ldots$, be as described in the preceding section. Let the positive integers t and k be such that*

$$|\lambda_t| > |\lambda_{t+1}| \text{ and } k = \sum_{j=1}^{t} (p_j + 1) = \sum_{j=1}^{t} \omega_j. \tag{3.1}$$

Determine the coefficients $c_j^{(n,k)}, j = 0, 1, \ldots, k$, for one of the procedures SMPE, SMMPE, *and* STEA, *by utilizing $u_n, u_{n+1}, \ldots$, as described in* (1.4) *and* (1.5). *Then, under the additional conditions given in* (2.8) *and* (2.9),

$$\hat{Q}_{n,k}(\lambda) \equiv \sum_{j=0}^{k} c_j^{(n,k)} \lambda^j = \prod_{j=1}^{t} (\lambda - \lambda_j)^{\omega_j} + O(\varepsilon(n)) \text{ as } n \to \infty, \tag{3.2}$$

where

$$\varepsilon(n) = n^{\alpha} \left| \frac{\lambda_{t+1}}{\lambda_t} \right|^n, \tag{3.3}$$

α being some nonnegative integer. In fact, if the λ_j whose moduli are $|\lambda_t|$ are simple, then $\alpha = \bar{p}$, where $\bar{p} = \max\{p_j : |\lambda_j| = |\lambda_{t+1}|\}$. Consequently, the polynomial $\hat{Q}_{n,k}(\lambda)$ for $n \to \infty$, has ω_j zeros $\lambda_{jl}(n), 1 \le l \le \omega_j$, that tend to $\lambda_j, j = 1, 2, \ldots, t$. For each j and l we have

$$\lambda_{jl}(n) - \lambda_j = O(\delta_j(n)^{1/\omega_j}) \text{ as } n \to \infty, \tag{3.4}$$

where

$$\delta_j(n) = n^{\bar{p}} \left| \frac{\lambda_{t+1}}{\lambda_j} \right|^n. \tag{3.5}$$

Let us denote

$$\hat{\lambda}_j(n) = \frac{1}{\omega_j} \sum_{l=1}^{\omega_j} \lambda_{jl}(n) \text{ or } \hat{\lambda}_j(n) = \left[\frac{1}{\omega_j} \sum_{l=1}^{\omega_j} \lambda_{jl}(n)^{-1} \right]^{-1}. \tag{3.6}$$

Then

$$\hat{\lambda}_j(n) - \lambda_j = O(\delta_j(n)) \text{ as } n \to \infty. \tag{3.7}$$

Also, the p_jth derivative of $\hat{Q}_{n,k}(\lambda)$ has exactly one zero $\tilde{\lambda}_j(n)$ that tends to λ_j and satisfies

$$\tilde{\lambda}_j(n) - \lambda_j = O(\delta_j(n)) \text{ as } n \to \infty. \tag{3.8}$$

Let the matrix A be normal, i.e., $AA^* = A^*A$. Then $p_j = 0$ hence $\omega_j = 1$ for all j. If the $c_j^{(n,k)}$ are determined through the procedures SMPE *and* STEA *with the standard Euclidean inner product, and k is such that*

$$|\lambda_k| > |\lambda_{k+1}|, \tag{3.9}$$

and provided $q = u_n$ for STEA, *then* (3.2) *and* (3.4) *are substantially improved to read, respectively,*

$$\hat{Q}_{n,k}(\lambda) = \prod_{j=1}^{k}(\lambda - \lambda_j) + O\left(\left|\frac{\lambda_{k+1}}{\lambda_k}\right|^{2n}\right) \text{ as } n \to \infty, \tag{3.10}$$

and, for $j = 1, \ldots, k$,

$$\lambda_j(n) - \lambda_j = O\left(\left|\frac{\lambda_{k+1}}{\lambda_j}\right|^{2n}\right) \text{ as } n \to \infty, \tag{3.11}$$

where $\lambda_j(n)$ is the unique zero of $\hat{Q}_{n,k}(\lambda)$ that tends to λ_j.

We note again that the result in (3.2) and (3.3) was originally given in [SiB, §6, Thm. 6.1], and those in (3.10) and (3.11) were originally given for SMPE in [Si3]. The rest of Theorem 3.1 is new in that it has appeared only recently in [Si6].

One important aspect of Theorem 3.1 is the construction of *optimal* approximations to *defective* eigenvalues through (3.6) and (3.7). From (3.4) it is clear that when $p_j = 0$ hence $\omega_j = 1$, which occurs automatically if λ_j is a nondefective eigenvalue, the rate of convergence of the approximation corresponding to λ_j is optimal. In case that λ_j is a defective eigenvalue and $p_j > 0$, the rate of convergence of each of its ω_j corresponding approximations is $1/\omega_j$ of the optimal rate. For this case (3.6) and (3.7) show how the poor approximations $\lambda_{jl}(n)$ can be combined in a simple way to give an optimal approximation, namely $\hat{\lambda}_j(n)$. Similarly, (3.8) shows that $\tilde{\lambda}_j(n)$, the zero of the p_jth derivative of $\hat{Q}_{n,k}(\lambda)$ that tends to λ_j, has the same optimal convergence rate as $\hat{\lambda}_j(n)$. The results in (3.10) and (3.11) show that the approximations obtained from SMPE and STEA for a normal matrix converge twice as fast as those obtained for a nonnormal diagonalizable matrix having the same spectrum.

Another important aspect of Theorem 3.1 is that it shows clearly that the quality of the approximations to $\lambda_1, \lambda_2, \ldots,$ is better when k is larger. To see this let us consider the two different cases in which $(k,t) = (k',t')$ and $(k,t) = (k'',t'')$ in (3.1) of Theorem 3.1, where $t' < t''$. Obviously, $|\lambda_{t'}| > |\lambda_{t''}|$, and also $|\lambda_{t'+1}| > |\lambda_{t''+1}|$. Consequently, $|\lambda_{t''+1}/\lambda_j| < |\lambda_{t'+1}/\lambda_j|$ for $j = 1, 2, \ldots$. The validity of our claim now follows by comparing the outcomes of (3.2)–(3.11) with $(k,t) = (k',t')$ and $(k,t) = (k'',t'')$.

Finally, as has already been mentioned in [SiB], the methods contained in Theorem 3.1 reduce precisely to the classical power methods when $k = 1$. Specifically, solving (1.4) with $k = 1$, we have $\hat{Q}_{n,1}(\lambda) = \lambda - u_{01}/u_{00}$, from which there follows $\rho(n) = u_{01}/u_{00}$ as the approximation to the largest eigenvalue of A. Now $\rho(n) = (u_n, u_{n+1})/(u_n, u_n) = (u_n, Au_n)/(u_n, u_n)$ for SMPE procedure and this is simply the Rayleigh quotient for u_n. Similarly, $\rho(n) = (q_1, Au_n)/(q_1, u_n)$ and $\rho(n) = (q, Au_n)/(q, u_n)$, respectively, for SMMPE and STEA procedures, and this is how the standard power method is defined.

3.2. Treatment of invariant subspace approximations. For the treatment of the eigenvectors and invariant subspaces we need some preliminary work.

Let us rewrite (2.6) in the form

$$F(z) = \sum_{j=1}^{M} \sum_{i=0}^{p_j} \frac{d_{ji}}{(z - z_j)^{i+1}} + G(z), \tag{3.12}$$

where

$$z_j = \lambda_j^{-1} \text{ and } d_{ji} = (-z_j)^{i+1} a_{ji} \text{ for all } j, i. \tag{3.13}$$

Thus the d_{ji} are the coefficients of the principal part of the Laurent expansion of $F(z)$ about the pole $z_j, j = 1, \ldots, M$.

Consider the rational function

$$\hat{F}(z) = \frac{F(z) - F_{n+\nu}(z)}{z^{n+\nu+1}}, \tag{3.14}$$

which is analytic at $z = 0$ and has the Maclaurin series expansion

$$\hat{F}(z) = \sum_{i=0}^{\infty} u_{n+\nu+i+1} z^i. \tag{3.15}$$

By (3.12) we can write

$$\hat{F}(z) = \sum_{i=0}^{p_j} \frac{\hat{d}_{ji}}{(z - z_j)^{i+1}} + \hat{G}_j(z), \tag{3.16}$$

where

$$\hat{d}_{ji} = z_j^{-n-\nu-1} \sum_{l=i}^{p_j} \binom{-n-\nu-1}{l-i} z_j^{-l+i} d_{jl}, \tag{3.17}$$

and $\hat{G}_j(z)$ is analytic at z_j, i.e., as above, the $\hat{d}_{ji}$ are coefficients of the principal part of the Laurent expansion of $\hat{F}(z)$ about the pole $z_j, j = 1, \ldots, M$. Unlike before, both $\hat{F}(z)$ and the $\hat{d}_{ji}$ depend on n, in addition. The vector $\hat{d}_{jp_j}$, being a scalar multiple of the constant vector d_{jp_j}, is an eigenvector of A corresponding to the eigenvalue λ_j. For $i \neq p_j$, the vector $\hat{d}_{ji}$, being a linear combination of the constant vectors $d_{jl}, i \leq l \leq p_j$, is in the invariant subspace Y_i, and, as is obvious from (3.17), the coefficients of the d_{jl} in this linear combination are polynomials in n, up to the common multiplicative factor $z_j^{-n-\nu-1}$.

Following now the developments in §5 of [Si6], we obtain the following constructive result for the $\hat{d}_{ji}$.

THEOREM 3.2. *With the notation and conditions of Theorem* 3.1, *let us define, for* $1 \leq j \leq t$,

$$\zeta_j(n) = 1/\hat{\lambda}_j(n) \text{ or } \zeta_j(n) = 1/\tilde{\lambda}_j(n), \tag{3.18}$$

and, for $0 \le i \le p_j$ *and* $1 \le l \le \omega_j$,

$$\hat{d}_{ji,l}(n) = (z - \zeta_j(n))^i \left. \frac{\sum_{r=1}^{k} c_r^{(n,k)} z^{k-r} \sum_{m=1}^{r} u_{n+\nu+m} z^{m-1}}{\sum_{r=0}^{k} c_r^{(n,k)} (k-r) z^{k-r-1}} \right|_{z=1/\lambda_{jl}(n)} \tag{3.19}$$

and

$$\hat{d}_{ji}(n) = \sum_{l=1}^{\omega_j} \hat{d}_{ji,l}(n). \tag{3.20}$$

Then, for $0 \le i \le p_j$, $\hat{d}_{ji}(n)$ *is an approximation to* $\hat{d}_{ji}$ *in* (3.17) *in the sense*

$$\limsup_{n\to\infty} |\hat{d}_{ji}(n) - \hat{d}_{ji}|^{1/n} \le |\lambda_{t+1}|. \tag{3.21}$$

We note that Theorem 3.2 actually contains the basic ingredients of a potentially bona fide numerical method for approximating the eigenvectors and other vectors in invariant subspaces corresponding to largest eigenvalues of A. The resulting method, which is described below, (i) makes use of only $u_n, u_{n+1}, \ldots$, disregarding $u_0, u_1, \ldots, u_{n-1}$ entirely, and (ii) enables us to construct optimal approximations to the vectors $a_{ji}, 0 \le i \le p_j$, for $p_j = 0$ as well as $p_j > 0$. We now turn to these constructions.

3.2.1. Approximation of the eigenvector a_{jp_j}. Let us first specialize the result of Theorem 3.2 to the case $i = p_j$. We have

$$\hat{d}_{jp_j} = \lambda_j^{n+\nu+1} d_{jp_j}, \tag{3.22}$$

so that (3.21) can also be written as

$$\limsup_{n\to\infty} |\lambda_j^{-n-\nu-1} \hat{d}_{jp_j}(n) - d_{jp_j}|^{1/n} \le \left| \frac{\lambda_{t+1}}{\lambda_j} \right|. \tag{3.23}$$

This clearly shows that the vector $\hat{d}_{jp_j}(n)$, as $n \to \infty$, aligns itself with the *constant* vector d_{jp_j}, which is proportional to the eigenvector a_{jp_j}, practically at the rate of $|\lambda_{t+1}/\lambda_j|^n$. It is thus sufficient to compute the vectors $\hat{d}_{ji,l}(n), 1 \le l \le \omega_j$, by (3.19), and then to form $\hat{d}_{ji}(n)$ by (3.20) as our approximation to the (appropriately normalized) eigenvector a_{jp_j}, and this is valid whether $p_j = 0$ or $p_j > 0$.

3.2.2. Approximation of the vectors $a_{ji}, 0 \le i \le p_j - 1$. Although the vector a_{jp_j} (up to a multiplicative constant) can be determined from $\hat{d}_{jp_j}(n)$ in a rather painless manner, the determination of the remaining a_{ji} from the $\hat{d}_{jl}(n)$ becomes somewhat involved. The reason for this is that the vectors $\hat{d}_{ji}$, apart from the scalar multiplicative factor $z_j^{-n-\nu-1}$, are linear combinations of the d_{jl} hence of the $a_{jl}, i \le l \le p_j$, with coefficients that vary as functions of n, as can be seen from (3.17) and (3.13), and as has been mentioned before. This means that the $\hat{d}_{ji}$ do *not* have a fixed direction with varying n.

Let us now rewrite (3.17) in the form

$$T(n) \begin{bmatrix} d_{j0} \\ d_{j1} \\ \vdots \\ d_{jp_j} \end{bmatrix} = z_j^{n+\nu+1} \begin{bmatrix} \hat{d}_{j0} \\ \hat{d}_{j1} \\ \vdots \\ \hat{d}_{jp_j} \end{bmatrix}, \tag{3.24}$$

where $T(n)$ is the upper triangular matrix

$$T(n) = \begin{bmatrix} \tau_{00} & \tau_{01} & \cdots & \tau_{0p_j} \\ & \tau_{11} & \cdots & \tau_{1p_j} \\ & & \ddots & \vdots \\ & & & \tau_{p_jp_j} \end{bmatrix}, \quad \tau_{il} = \binom{-n-\nu-1}{l-i} z_j^{-l+i} \quad \text{all } i \text{ and } l. \tag{3.25}$$

Obviously, $T(n)$ is invertible since its diagonal elements are unity. Thus,

$$\begin{bmatrix} d_{j0} \\ d_{j1} \\ \vdots \\ d_{jp_j} \end{bmatrix} = T(n)^{-1} \begin{bmatrix} \hat{d}_{j0} \\ \hat{d}_{j1} \\ \vdots \\ \hat{d}_{jp_j} \end{bmatrix} z_j^{n+\nu+1}, \tag{3.26}$$

where $T(n)^{-1}$ is also upper triangular, its diagonal elements being unity.

Now since all elements of $T(n)$ are polynomials in n, and since its determinant is unity, the elements of $T(n)^{-1}$ turn out to be polynomials in n, i.e., the matrix $T(n)^{-1}$ can grow at most polynomially as $n \to \infty$. If we denote the nonzero elements of $T(n)^{-1}$ by $\rho_{il}, i \le l \le p_j, 0 \le i \le p_j$, then we can write (3.26) in the form

$$d_{ji} = z_j^{n+\nu+1} \sum_{l=i}^{p_j} \rho_{il} \hat{d}_{jl}, \quad 0 \le i \le p_j. \tag{3.27}$$

Let us replace $\hat{d}_{jl}$ in (3.27) by $[(\hat{d}_{jl} - \hat{d}_{jl}(n)) + \hat{d}_{jl}(n)]$, and invoke (3.21). After some manipulation we obtain

$$\limsup_{n\to\infty} \left| d_{ji} - z_j^{n+\nu+1} \sum_{l=i}^{p_j} \rho_{il} \hat{d}_{jl}(n) \right|^{1/n} \le \left| \frac{\lambda_{t+1}}{\lambda_j} \right|. \tag{3.28}$$

This implies that the vector $\sum_{l=i}^{p_j} \rho_{il} \hat{d}_{jl}(n)$ aligns itself with the fixed vector d_{ji} as $n \to \infty$ practically at the rate of $|\lambda_{t+1}/\lambda_j|^n$. We leave the details of the proof of (3.28) to the reader.

We note that (3.28) shows how to construct a good approximation to d_{ji} from the $\hat{d}_{jl}(n)$ and λ_j, provided λ_j is known. Since λ_j is not known, however, the vector $\sum_{l=i}^{p_j} \rho_{il} \hat{d}_{jl}(n)$ cannot be constructed. We, therefore, propose to replace λ_j in the matrix $T(n)^{-1}$ by the known approximations $\zeta_j(n)$. Also, in this case, it can be shown that (3.28) remains valid. Again, we leave the details of the proof to the reader.

Before closing this section, we must mention that the developments of this section are meant to be theoretical in general. Although they can be used for computational purposes for small values of k, their use for large k is likely to introduce numerical instabilities in many cases. These instabilities are mainly a result of our direct use of the power iterations $u_{n+i} = A^i u_n, i = 0, 1, \ldots$. They exhibit themselves first of all through the poor computed approximations to the λ_j, which ultimately affect the computed eigenvector approximations. This problem can be remedied by observing that the approximations $F_{n,k}(z)$ that we developed and applied to the matrix eigenvalue problem are very tightly connected with Krylov subspace methods for some of which there exist computationally stable implementations. In particular, the SMPE and

STEA procedures are related to the method of Arnoldi and the method of Lanczos, respectively, as we show in detail in the next two sections.

4. General projection methods and the methods of Arnoldi and Lanczos for the matrix eigenproblem.

4.1. General projection methods. Let $\{v_1, \ldots, v_k\}$ and $\{w_1, \ldots, w_k\}$ be two linearly independent sets of vectors in $\mathbf{C}^N$, and define the $N \times k$ matrices V and W by

$$V = [v_1|v_2|\cdots|v_k] \text{ and } W = [w_1|w_2|\cdots|w_k]. \tag{4.1}$$

In addition, let us agree to denote the subspaces span $\{v_1, \ldots, v_k\}$ and span $\{w_1, \ldots, w_k\}$ by V and W, respectively. For simplicity, let us also take (x, y) to be the standard Euclidean inner product x^*y.

In projection methods one looks for an approximate eigenvalue-eigenvector pair (λ, x) with $x \in V$ that satisfies the condition

$$(y, Ax - \lambda x) = 0 \quad \text{for all } y \in W, \tag{4.2}$$

which can also be written in the equivalent form

$$W^*(A - \lambda I)V\xi = 0 \quad \text{for some } \xi \in \mathbf{C}^k. \tag{4.3}$$

Here we have used the fact that $x \in V$ implies that $x = V\xi$ for some $\xi \in \mathbf{C}^k$. Of course, (4.3) holds if and only if λ is an eigenvalue of the matrix pencil (W^*AV, W^*V), i.e., it satisfies the characteristic equation

$$\det(W^*AV - \lambda W^*V) = 0. \tag{4.4}$$

In general, (4.4) has k solutions for λ, which are known as *Ritz values* in the literature. Given that λ' is a Ritz value, the corresponding eigenvector ξ' is a solution of the homogeneous system in (4.3). The eigenvector approximation corresponding to λ' is now $x' = V\xi'$, and is known as a *Ritz vector.*

The different projection methods are characterized by the subspaces V and W that they employ. (Note that V and W are also called, respectively, the right and left subspaces.)

4.2. The method of Arnoldi. In this method V and W are Krylov subspaces given by

$$V = V_{k-1} = \text{ span}\{u_0, Au_0, \ldots, A^{k-1}u_0\} \quad \text{and} \quad W = W_{k-1} = V_{k-1}, \tag{4.5}$$

for some arbitrary vector u_0.

Arnoldi has given a very successful implementation of this method. In this implementation the vectors $A^iu_0, i = 0, 1, \ldots$, are orthogonalized by a very special Gram–Schmidt process as follows:

Step 0. Let $v_1 = u_0/\|u_0\|$.

Step 1. For $j = 1, \ldots, k-1$, do

(4.6) Determine the scalar $h_{j+1,j} > 0$ and the vector v_{j+1}, such that $h_{j+1,j}v_{j+1} = Av_j - \sum_{i=1}^{j} h_{ij}v_i, h_{ij} = (v_i, Av_j), 1 \le i \le j$, and $\|v_{j+1}\| = 1$.

Thus the $N \times k$ matrix $V = [v_1|v_2|\cdots|v_k]$ is unitary in the sense that V^*V is the $k \times k$ identity matrix. As a result, $W^*V = V^*V = I$, and the generalized eigenvalue problem of (4.3) now becomes

$$H\xi = \lambda\xi, \tag{4.7}$$

where H is the $k \times k$ upper Hessenberg matrix

$$H = \begin{bmatrix} h_{11} & h_{12} & \cdots & & h_{1k} \\ h_{21} & h_{22} & \cdots & & h_{2k} \\ & h_{32} & \cdots & & h_{3k} \\ & & \ddots & & \vdots \\ & & & h_{k,k-1} & h_{kk} \end{bmatrix}, \tag{4.8}$$

i.e., the Ritz values are the eigenvalues of H.

4.3. The method of Lanczos. In this method V and W are the Krylov subspaces

$$\begin{aligned} V &= V_{k-1} = \operatorname{span}\{u_0, Au_0, \ldots, A^{k-1}u_0\} \quad \text{and} \\ W &= W_{k-1} = \operatorname{span}\{q, A^*q, \ldots, (A^*)^{k-1}q\}, \end{aligned} \tag{4.9}$$

for some arbitrary vectors u_0 and q.

The algorithm given by Lanczos generates one set of vectors $\{v_1, \ldots, v_k\}$ from the $A^iu_0, i = 0, 1, \ldots, k-1$, and another set of vectors $\{w_1, \ldots, w_k\}$ from the $(A^*)^iq, i = 0, 1, \ldots, k-1$, that satisfy the biorthogonality condition

$$(w_i, v_j) = \delta_{ij}, \tag{4.10}$$

as long as the process does not break down. This is achieved by the following algorithm.

Step 0. Set $v_1 = \sigma u_0$ and $w_1 = \tau q$ such that $(w_1, v_1) = 1$.

Step 1. For $j = 1, \ldots, k-1$, do

(4.11) (a) Compute $\hat{v}_{j+1}$ and $\hat{w}_{j+1}$ by
$\hat{v}_{j+1} = Av_j - \alpha_j v_j - \beta_j v_{j-1}$ and $\hat{w}_{j+1} = A^*w_j - \bar{\alpha}_j w_j - \bar{\delta}_j w_{j-1}$, with
$\alpha_j = (w_j, Av_j)$. (When $j = 1$ take $\beta_1 v_0 = \bar{\delta}_1 w_0 = 0$.)
(b) Choose δ_{j+1} and β_{j+1} such that
$\delta_{j+1}\beta_{j+1} = (\hat{w}_{j+1}, \hat{v}_{j+1})$, and set
$v_{j+1} = \hat{v}_{j+1}/\delta_{j+1}$ and $w_{j+1} = \hat{w}_{j+1}/\bar{\beta}_{j+1}$.

By (4.10) the matrices V and W satisfy $W^*V = I$. As a result, the generalized eigenvalue problem of (4.3) becomes

$$H\xi = \lambda\xi, \tag{4.12}$$

where H is the $k \times k$ tridiagonal matrix

$$H = \begin{bmatrix} \alpha_1 & \beta_2 & & & & \\ \delta_2 & \alpha_2 & \beta_3 & & & \\ & \delta_3 & \alpha_3 & \beta_4 & & \\ & & \ddots & \ddots & \ddots & \\ & & & & & \beta_k \\ & & & & \delta_k & \alpha_k \end{bmatrix}, \tag{4.13}$$

and the Ritz values are the eigenvalues of H.

4.4. The case of Hermitian A. The subspaces V in (4.5) and (4.9) are identical. When A is Hermitian, i.e., $A^* = A$, and $q = u_0$, the subspaces W in (4.5) and (4.9) become identical too. Thus the methods of Arnoldi and Lanczos become equivalent for the case under consideration. Furthermore, it can be shown that the elements h_{ij} of the matrix H in the method of Arnoldi satisfy $\overline{h_{i,i+1}} = h_{i+1,i}$ so that $h_{i,i+1} = h_{i+1,i} > 0$ for $i = 1, 2, \ldots, k-1$, while $h_{ij} = 0$ for $j \geq i+2$. The diagonal elements h_{ii} are all real. That is to say, in the absence of roundoff, the matrix H is real symmetric tridiagonal. If we pick $q = u_0$ and choose $\delta_j = \beta_j = \sqrt{(\hat{v}_j, \hat{v}_j)}$ in the method of Lanczos, then the matrix H in (4.13) turns out to be real symmetric and is exactly the same as the one produced by the method of Arnoldi.

The properties of the Ritz values and Ritz vectors of the Lanczos method, as applied to Hermitian matrices, have been analyzed by Kaniel [K], Paige [Pai], and Saad [Sa1]. The paper [Sa2] gives results for non-Hermitian matrices.

5. Equivalence of rational approximation procedures and Krylov subspace methods. We now go back to the rational approximation procedures SMPE, SMMPE, and STEA. In particular, we concentrate on the poles and residues of the rational functions $F_{n,k}(z)$.

5.1. Poles of $F_{n,k}(z)$ vs. Ritz values. From the determinant representations of $F_{n,k}(z)$ that are given in Theorem 2.2 of [Si6], it follows that the denominator $Q_{n,k}(z)$ of $F_{n,k}(z)$ is a constant multiple of the determinant

$$D(\lambda) = \begin{vmatrix} 1 & \lambda & \ldots & \lambda^k \\ u_{00} & u_{01} & \ldots & u_{0k} \\ u_{10} & u_{11} & \ldots & u_{1k} \\ \vdots & \vdots & & \vdots \\ u_{k-1,0} & u_{k-1,1} & \ldots & u_{k-1,k} \end{vmatrix}, \tag{5.1}$$

where $\lambda = z^{-1}$ and u_{ij} are as defined in (1.5). This implies that the zeros of the polynomial $D(\lambda)$ are the reciprocals of the zeros of $Q_{n,k}(z)$, or, equivalently, the reciprocals of the poles of $F_{n,k}(z)$. In addition, they are the roots of a generalized eigenvalue problem as we show next.

THEOREM 5.1. *Whatever the u_{ij}, the zeros of the polynomial $D(\lambda)$ in* (5.1) *are the eigenvalues of the matrix pencil (X, T), where*

(5.2)

$$X = \begin{bmatrix} u_{01} & u_{02} & \cdots & u_{0k} \\ u_{11} & u_{12} & \cdots & u_{1k} \\ \vdots & \vdots & & \vdots \\ u_{k-1,1} & u_{k-1,2} & \cdots & u_{k-1,k} \end{bmatrix} \quad \textit{and} \quad T = \begin{bmatrix} u_{00} & u_{01} & \cdots & u_{0,k-1} \\ u_{10} & u_{11} & \cdots & u_{1,k-1} \\ \vdots & \vdots & & \vdots \\ u_{k-1,0} & u_{k-1,1} & \cdots & u_{k-1,k-1} \end{bmatrix},$$

i.e., they satisfy the equation

$$\det(X - \lambda T) = 0. \tag{5.3}$$

Proof. Multiply the $(j-1)$st column of $D(\lambda)$ by λ and subtract from the jth column for $j = k+1, k, \ldots, 2$, in this order. This results in

$$D(\lambda) = \left|\begin{array}{c|c} 1 & 0\cdots 0 \\ \hline u_{00} & \\ u_{10} & X - \lambda T \\ \vdots & \\ u_{k-1,0} & \end{array}\right| = \det(X - \lambda T), \tag{5.4}$$

thus proving the claim. □

In the remainder of this section we take $(x, y) = x^*y$.

When u_{ij} are as in (1.5), Theorem 5.1 takes on the following interesting form.

THEOREM 5.2. *Define the $N \times k$ matrices V and W by*

$$V = [u_n | u_{n+1} | \cdots | u_{n+k-1}] \tag{5.5}$$

and

$$\begin{aligned} &W = V \text{ for SMPE}, \\ &W = [q_1 | q_2 | \cdots | q_k] \text{ for SMMPE}, \\ &W = [q | A^*q | \cdots | (A^*)^{k-1}q] \text{ for STEA}. \end{aligned} \tag{5.6}$$

Then, with u_{ij} as defined by (1.5), *the zeros of $D(\lambda)$ are the eigenvalues of the matrix pencil (W^*AV, W^*V), i.e., they satisfy*

$$\det(W^*AV - \lambda W^*V) = 0. \tag{5.7}$$

Consequently, the reciprocals of the poles of the rational approximations $F_{n,k}(z)$ obtained from the SMPE *or* SMMPE *or* STEA *procedures are the Ritz values of the Krylov subspace methods whose right and left subspaces are column spaces of V and W, respectively.*

Proof. Since Theorem 5.1 applies, all we need to show is that $X = W^*AV$ and $T = W^*V$ there. That $T = W^*V$ follows from (1.5), (5.2), (5.5), and (5.6). From (1.5), (5.2), and (5.6), we similarly have $X = W^*[u_{n+1} | \cdots | u_{n+k}]$. Now using the fact that $u_{j+1} = Au_j, j \geq 0$, we also have $[u_{n+1} | \cdots | u_{n+k}] = AV$. Consequently, $X = W^*AV$. Again, from $u_{j+1} = Au_j, j \geq 0$, we realize, in addition, that the right subspace for all three methods is none other than the Krylov subspace span $\{u_n, Au_n, \ldots, A^{k-1}u_n\}$. This completes the proof. □

5.2. Residues of $F_{n,k}(z)$ vs. Ritz vectors. Turning Theorem 5.2 around, what we have is that the Ritz values obtained by applying the Krylov subspace methods whose left and right subspaces are column spaces of V and W, respectively, are, in fact, the reciprocals of the poles of the corresponding rational approximations $F_{n,k}(z)$ to the meromorphic function $F(z) = \sum_{i=0}^{\infty} u_i z^i$. An immediate question that arises is, of course, whether there is any connection between the Ritz *vectors* and the $F_{n,k}(z)$. The answer, which is in the affirmative, is provided in Theorem 5.3 below.

THEOREM 5.3. *Let $\hat{\lambda}$ be a Ritz value of the Krylov subspace methods whose right and left subspaces are column spaces of, respectively, V and W in Theorem* 5.2. *Denote the corresponding Ritz vector by $\hat{x}$. Let $\nu = -1$ in the corresponding rational approximation $F_{n,k}(z)$, cf.* (1.2). *Provided $\hat{\lambda}$ is simple, $\hat{x}$ is a constant multiple of the residue of $F_{n,k}(z)$ at the pole $\hat{z} = 1/\hat{\lambda}$.*

Proof. Let us first determine the residue of $F_{n,k}(z)$ at the pole $\hat{z} = 1/\hat{\lambda}$. With $\nu = -1$

$$\text{Res } F_{n,k}(z)|_{z=\hat{z}} = \frac{P_{n,k}(\hat{z})}{Q'_{n,k}(\hat{z})} = \frac{\sum_{r=0}^{k} c_r \hat{z}^{k-r} F_{n+r-1}(\hat{z})}{Q'_{n,k}(\hat{z})}, \tag{5.8}$$

since $Q'_{n,k}(\hat{z}) \neq 0$ that follows from the assumption that $\hat{\lambda}$ is simple, which implies that $\hat{z}$ is a simple pole. By $F_{n+s}(z) = F_{n-1}(z) + \sum_{m=n}^{n+s} u_m z^m$ and $\sum_{r=0}^{k} c_r \hat{z}^{k-r} = 0$, we can rewrite (5.8) in the form

$$\text{Res } F_{n,k}(z)|_{z=\hat{z}} = \frac{1}{Q'_{n,k}(\hat{z})} \sum_{r=1}^{k} c_r \hat{z}^{k-r} \sum_{m=n}^{n+r-1} u_m \hat{z}^m = \frac{\hat{z}^{n+k-1}}{Q'_{n,k}(\hat{z})} \sum_{m=0}^{k-1} \eta_m u_{n+m}, \tag{5.9}$$

where

$$\eta_m = \sum_{r=m+1}^{k} c_r \hat{\lambda}^{r-m-1}, \qquad m = 0, 1, \ldots, k-1. \tag{5.10}$$

Let us now denote $\eta = (\eta_0, \eta_1, \ldots, \eta_{k-1})^T$. Then (5.9) implies that Res $F_{n,k}(z)|_{z=\hat{z}}$ is a scalar multiple of $V\eta$. Recall that the Ritz vector corresponding to $\hat{\lambda}$ is $V\hat{\xi}$, where $\hat{\xi} \in C^k$ and satisfies $W^*(A - \hat{\lambda}I)V\hat{\xi} = 0$, which, on account of Theorem 5.2, is the same as $(X - \hat{\lambda}T)\hat{\xi} = 0$. Thus in order to show that Res $F_{n,k}(z)|_{z=\hat{z}}$ is a constant multiple of the Ritz vector corresponding to the Ritz value $\hat{\lambda}$, it is sufficient to show that

$$(X - \hat{\lambda}T)\eta = 0. \tag{5.11}$$

From (5.2), the $(i+1)$st component of the k-dimensional vector $\tau = (X - \hat{\lambda}T)\eta, i = 0, 1, \ldots, k-1$, is

$$\tau_i = \sum_{m=0}^{k-1} (u_{i,m+1} - \hat{\lambda} u_{im}) \eta_m, \tag{5.12}$$

which, by (5.10), becomes

$$\tau_i = \sum_{m=0}^{k-1} (u_{i,m+1} - \hat{\lambda} u_{im}) \sum_{r=m+1}^{k} c_r \hat{\lambda}^{r-m-1}. \tag{5.13}$$

Expanding and rearranging this summation, we obtain

$$\tau_i = -u_{i0} \left(\sum_{r=1}^{k} c_r \hat{\lambda}^r \right) + \sum_{m=1}^{k} u_{im} c_m. \tag{5.14}$$

Recalling that $\sum_{r=0}^{k} c_r \hat{\lambda}^r = 0$, we can rewrite (5.14) as

$$\tau_i = \sum_{m=0}^{k} u_{im} c_m. \tag{5.15}$$

Finally, from the assumption that $c_k = 1$ and from the fact that $c_0, c_1, \ldots, c_{k-1}$ satisfy the linear equations in (1.4), we conclude that

$$\tau_i = 0, \quad i = 0, 1, \ldots, k-1. \tag{5.16}$$

This completes the proof. □

5.3. Summary of $F_{n,k}(z)$ vs. Krylov subspace methods. We now combine the results of Theorems 5.2 and 5.3 to state the following equivalence theorem, which forms the main result of this section, and one of the main results of this work.

THEOREM 5.4. *Let $F_{n,k}(z)$ be the rational approximation obtained by applying the* SMPE *or* SMMPE *or* STEA *procedure to the vector-valued power series $\sum_{m=0}^{\infty} u_m z^m$, where $u_m = A^m u_0, m = 0, 1, \ldots$, are power iterations. Denote the reciprocals of the poles of $F_{n,k}(z)$ by $\lambda'_1, \ldots, \lambda'_k$. Setting $\nu = -1$ in the numerator of $F_{n,k}(z)$, denote the corresponding residues of $F_{n,k}(z)$ by $x'_1, \ldots, x'_k$. Next, denote by $\lambda''_1, \ldots, \lambda''_k$ and $x''_1, \ldots, x''_k$, respectively, the Ritz values and corresponding Ritz vectors produced by the Krylov subspace methods whose right subspace is* $\operatorname{span}\{u_n, Au_n, \ldots, A^{k-1}u_n\}$ *and left subspaces are the column spaces of the matrices W in* (5.6). *Then*

$$\lambda'_j = \lambda''_j, \qquad j = 1, \ldots, k, \tag{5.17}$$

and

$$x'_j \propto x''_j, \text{ provided } \lambda'_j \text{ is simple.} \tag{5.18}$$

More can be said about the SMPE and STEA procedures versus the methods of Arnoldi and Lanczos, and this is done in Corollary 5.5 below.

COROLLARY 5.5. *With $F_{n,k}(z), \lambda'_j, x'_j, j = 1, \ldots, k$, as in Theorem* 5.4, *let λ''_j, x''_j, $j = 1, \ldots, k$, be the Ritz values and Ritz vectors produced by applying the k-step Arnoldi or Lanczos methods to the matrix A, starting with the vector $u_n = A^n u_0$. (That is to say, replace the initial vector u_0 in Step* 0 *of* (4.6) *or* (4.11) *by the nth power iteration u_n.) In addition, let q be the same vector for the* STEA *procedure and the Lanczos method. Then the* SMPE *and* STEA *procedures are equivalent to the methods of Arnoldi and Lanczos, respectively, precisely in the sense of* (5.17) *and* (5.18).

Now that we have shown the equivalence of the methods of Arnoldi and Lanczos with the generalized power methods based on the SMPE and STEA approximation procedures, we realize that those results we proved in §3 for the latter and which pertain to the nondefective as well as defective eigenvalues of A are, in fact, new results for the former. That is to say, if we apply the methods of Arnoldi or Lanczos of order k to the matrix A starting with the nth power iteration $u_n = A^n u_0$ for large n, then the Ritz values are approximations to the k largest distinct eigenvalues of A counted according to the multiplicities that appear in (2.2). Similarly, the Ritz vectors can be used for constructing the approximations to the corresponding invariant subspaces. These points will be considered in greater detail in the next section.

Judging from Theorems 3.1 and 3.2, we conclude that applying Krylov subspace methods beginning with $u_n = A^n u_0, n > 0$, rather than with u_0, may be advantageous, especially when the eigenvalues that are largest in modulus *and* the corresponding eigenvectors and invariant subspaces are needed. Specifically, a given level of accuracy may be achieved for smaller values of k as n is increased. We recall that k is also the number of vectors $v_1, v_2, \ldots$, in (4.1) that need to be saved. Thus we see that the strategy in which Krylov subspace methods are applied to u_n with n sufficiently large

may result in substantial savings in storage. In addition, smaller k means savings in the computational overhead caused by the arithmetic operations that lead to the matrices V and W, and, subsequently, to the Ritz vectors. (For a detailed discussion of this point we refer the reader to §7 Example 7.2.) All this was observed to be the case in various examples done by the author.

5.4. Optimality properties of the Arnoldi method. In §1 we mentioned that the coefficients of $c_i^{(n,k)}$ of the denominator polynomial $Q_{n,k}(z)$ of $F_{n,k}(z)$ for the SMPE procedure are the solution to the optimization problem given in (1.6). If we now pick the vectors u_m as the power iterations $u_m = A^m u_0, m = 0, 1, \ldots$, then (1.6) reads

$$\min_{c_0, c_1, \ldots, c_{k-1}} \left\| \left(\sum_{j=0}^{k-1} c_j A^j + A^k \right) u_n \right\|. \tag{5.19}$$

Exploiting the fact that the method of Arnoldi is equivalent to the generalized power method based on the SMPE approximation procedure, we can state the following optimality properties for the Arnoldi method as applied to a *general* matrix A.

THEOREM 5.6. *Let $\lambda_j', x_j', j = 1, 2, \ldots, k$, be the Ritz values and appropriately normalized Ritz vectors, respectively, produced by applying the k-step Arnoldi method to the matrix A starting with the power iteration $u_n = A^n u_0$. Let $\mathcal{P}_k$ denote the set of monic polynomials of degree exactly k, while π_k denotes the set of polynomials of degree at most k. Then for $k < k_0$, cf.* (2.4),

$$\left\| \left[\prod_{i=1}^{k} (A - \lambda_i' I) \right] u_n \right\| = \min_{f \in \mathcal{P}_k} \|f(A) u_n\| \equiv \varepsilon_{n,k}, \tag{5.20}$$

$$x_j' = \left[\prod_{\substack{i=1 \\ i \neq j}}^{k} (A - \lambda_i' I) \right] u_n, \tag{5.21}$$

$$(A - \lambda_j' I) x_j' = \left(\sum_{i=0}^{k-1} c_i^{(n,k)} A^i + A^k \right) u_n = \sum_{i=0}^{k-1} c_i^{(n,k)} u_{n+i} + u_{n+k}, \tag{5.22}$$

$$\begin{aligned} \|(A - \lambda_j' I) x_j'\| &= \min_{\lambda \in \mathbf{C}, g \in \mathcal{P}_{k-1}} \|(A - \lambda I) g(A) u_n\|, \\ &= \min_{\lambda \in \mathbf{C}} \|(A - \lambda I) x_j'\|, \\ &= \min_{g \in \mathcal{P}_{k-1}} \|(A - \lambda_j' I) g(A) u_n\|, \\ &= \varepsilon_{n,k} \text{ independently of } j, \end{aligned} \tag{5.23}$$

and

$$((A - \lambda_j' I) x_j', g(A) u_n) = 0 \quad \text{all } g \in \pi_{k-1}. \tag{5.24}$$

For $k = k_0$, we have $A x_j' = \lambda_j' x_j'$.

Proof. We start by noting that (5.24) is nothing but a restatement of the requirement that $Ax'_j - \lambda'_j x'_j$ be orthogonal to the left subspace of the Arnoldi method, which is also its right subspace $V = \{g(A)u_n : g \in \pi_{k-1}\}$.

Since the Ritz values $\lambda'_j, j = 1, \dots, k$, are the zeros of the monic polynomial $\hat{Q}_{n,k}(\lambda) = \sum_{i=0}^{k-1} c_i^{(n,k)} \lambda^i + \lambda^k$, we can write

$$\hat{Q}_{n,k}(\lambda) = \prod_{i=1}^{k} (\lambda - \lambda'_i). \tag{5.25}$$

Thus

$$\hat{Q}_{n,k}(A) = \sum_{i=0}^{k-1} c_i^{(n,k)} A^i + A^k = \prod_{i=1}^{k} (A - \lambda'_i I). \tag{5.26}$$

Combining (5.26) with (5.19), we obtain (5.20).

Provided x'_j is as given by (5.21), the proofs of (5.22) and (5.23) are immediate.

To prove the validity of (5.21) it is sufficient to show that $x'_j \in V$ and that $(A - \lambda'_j I)x'_j$ is orthogonal to all the vectors in V. That $x'_j \in V$ is obvious from (5.21) itself. The fact that $c_i^{(n,k)}, i = 0, 1, \dots, k-1$, are the solution of the optimization problem in (5.19) implies that the vector $\hat{Q}_{n,k}(A)u_n$ is orthogonal to every vector in V. But $\hat{Q}_{n,k}(A)u_n = (A - \lambda'_j I)x'_j$, as can be seen from (5.26). This completes the proof. □

Note that the proofs of (5.20) and (5.21) for Hermitian matrices can also be found in [Par2, Chap. 12, pp. 239–240].

A few historical notes on the methods of Arnoldi and Lanczos are now in order.

Following the work of Arnoldi the equivalent form in (5.19) was suggested in a paper by Erdelyi [E], in the book by Wilkinson [W, pp. 583–584], and in the papers by Manteuffel [M] and Sidi and Bridger [SiB]. The equivalence of the different approaches does not seem to have been noticed, however. For instance, [W] discusses both approaches without any attempt to explore the connection between them. With the exception of [SiB], these works all consider the case $n = 0$. The case $n > 0$ and the limit as $n \to \infty$ are considered in [SiB] and [Si3].

In his discussion of the power iterations in [H, Chap. 7], Householder gives determinantal representations of certain polynomials whose zeros are approximations to the largest eigenvalues of the matrix being considered. One of these representations, namely, the one given in (16) in [H, p. 186], coincides with the determinant $D(\lambda)$ in (5.1) of the present work pertaining to the STEA approximation procedure with $n \geq 0$. It is shown there that the zeros of $D(\lambda)$ tend to the k largest eigenvalues of the matrix A as $n \to \infty$, but a theorem as detailed as our Theorem 3.1 is not given. It is also mentioned in the same place that, apart from a constant multiplicative factor, the polynomials $D(\lambda)$ with $n = 0$ are precisely the so-called Lanczos polynomials given in (10) of [H, p. 23] that are simply $\det(\lambda I - H)$ with H as given in (4.13). As we pointed out in this section, up to a constant multiplicative factor, $D(\lambda)$ with $n > 0$ is itself the Lanczos polynomial $\det(\lambda I - H)$ when the Lanczos method is being applied with u_0 replaced by $u_n = A^n u_0$. It is not clear to the author whether this connection between $D(\lambda)$ with $n > 0$ and the Lanczos method has been observed before or not.

6. Stable numerical implementations. In this section we concentrate on the implementation of the generalized power methods based on the SMPE and the STEA

approximation procedures as these are related to the methods of Arnoldi and Lanczos, respectively, and as good implementations for the latter are known. For example, the implementations in (4.6) and (4.11) are usually quite stable.

6.1. General computational considerations. The theoretical results of §3 all involve the limiting procedure $n \to \infty$. When $|\lambda_1|$ is larger (smaller) than 1, we may have difficulties in implementing the procedures above due to possible overflow (underflow) in the computation of the vectors u_m for large m. This situation can be remedied easily as will be shown below.

We first observe that the denominator polynomial $Q_{n,k}(z)$ of the vector-valued rational approximation $F_{n,k}(z)$ remains unchanged when the vectors $u_n, u_{n+1}, u_{n+2}, \dots$, are all multiplied by the same scalar, say α, and so do its zeros. Consequently, the vectors $\hat{d}_{ji}(n)$ defined in Theorem 3.2 remain the same up to the multiplicative factor α. That is to say, as far as the matrix eigenvalue problem is concerned, multiplication of the vectors $u_n, u_{n+1}, \dots$, by the scalar α leaves the eigenvalue approximations unchanged and multiplies the eigenvector approximations by α.

For the purpose of numerical implementation we propose to pick $\alpha = 1/\|u_n\|$, and we achieve this by the following simple algorithm that is also used in the classical power method.

(6.1)
Step 0. Pick u_0 arbitrarily such that $\|u_0\| = 1$.
Step 1. For $m = 1, 2, \dots, n$, do
$w_m = Au_{m-1}$
$u_m = w_m/\|w_m\|$.

6.2. Treatment of defective eigenvalues. When the eigenvalue λ_j is defective and has $\omega_j > 1$ in (2.2), then, under the conditions of Theorem 3.1, there are precisely ω_j Ritz values $\lambda_{jl}(n), 1 \le l \le \omega_j$, that tend to λ_j, each with the rate of convergence $O([n^{\bar{p}}|\lambda_{t+1}/\lambda_j|^n]^{1/\omega_j})$ as $n \to \infty$. That is to say, the Ritz values for a defective eigenvalue are not as effective as the ones for nondefective eigenvalues. However, $\hat{\lambda}_j(n)$ and $\tilde{\lambda}_j(n)$ that are defined in Theorem 3.1 do enjoy the property that they tend to λ_j with the optimal rate of convergence $O(n^{\bar{p}}|\lambda_{t+1}/\lambda_j|^n)$ as $n \to \infty$, as in the case of a nondefective eigenvalue.

As for the invariant subspaces $Y_i, i = 0, 1, \dots, p_j, p_j = \omega_j - 1$, the most basic result to use is Theorem 3.2. According to this theorem and the subsequent developments, the building blocks for the invariant subspaces are the vectors $\hat{d}_{ji,l}(n)$ that are defined by (3.19). Now the vector $\hat{d}_{ji,l}(n)$ is a constant multiple of $\operatorname{Res} F_{n,k}(z)|_{z=z_{jl}(n)}$, where $z_{jl}(n) = 1/\lambda_{jl}(n)$, which, when $\nu = -1$, is a constant multiple of the Ritz vector corresponding to $\lambda_{jl}(n)$ by Theorem 5.4. That is, once the Ritz vectors have been computed, they can be used to construct the vectors $\hat{d}_{ji,l}(n)$ which, in turn, are used in constructing the approximate invariant subspaces Y_i with optimal accuracy.

Let us now show how the vector $\hat{d}_{ji,l}(n)$ is expressed in terms of the corresponding Ritz vector. For simplicity of notation we shall write $\hat{z} = z_{jl}(n) = 1/\lambda_{jl_{(n)}}$. The Ritz vector corresponding to $\lambda_{jl}(n)$ is $\hat{x} = \sum_{i=1}^{k} \xi_i v_i$, where $v_1 = u_n$ and $(u_n, u_n) = 1$ by (6.1). We recall that for the method of Arnoldi the vectors $v_1, v_2, \dots, v_k$ are actually the ones that would be obtained by orthogonalizing the power iterations $u_n, Au_n, \dots, A^{k-1}u_n$ by the Gram–Schmidt process. For the method of Lanczos the vectors $v_1, v_2, \dots, v_k$ are obtained by biorthogonalizing $u_n, Au_n, \dots, A^{k-1}u_n$ against the vectors $q, A^*q, \dots, (A^*)^{k-1}q$. In both cases we have

$$AV = VH + R, \tag{6.2}$$

where H is the upper Hessenberg matrix of (4.8) for the Arnoldi method or the tridiagonal matrix of (4.13) for the Lanczos method, and thus it is upper Hessenberg in both cases. The matrix R has all of its first $k-1$ columns equal to zero, and its kth column is $h_{k+1,k}v_{k+1}$.

From the way the vectors $v_1, v_2, \ldots, v_k$ are constructed it is easy to see that

$$V = [u_n | Au_n | \cdots | A^{k-1}u_n]B, \tag{6.3}$$

where B is the upper triangular matrix

$$B = \begin{bmatrix} \beta_{11} & \beta_{12} & \cdots & \beta_{1k} \\ & \beta_{22} & \cdots & \beta_{2k} \\ & & \ddots & \vdots \\ & & & \beta_{kk} \end{bmatrix}, \tag{6.4}$$

whose entries β_{ij} are required. Substituting (6.3) in (6.2), we have

$$[Au_n | A^2u_n | \cdots | A^ku_n]B = [u_n | Au_n | \cdots | A^{k-1}u_n]BH + R. \tag{6.5}$$

By equating the jth columns of both sides of (6.5) for $j < k$, we obtain

$$\sum_{i=1}^{j}(A^iu_n)\beta_{ij} = \sum_{i=0}^{j}(A^iu_n)(BH)_{i+1,j} \tag{6.6}$$

as the matrices B and BH are upper triangular and upper Hessenberg, respectively. From the linear independence of the vectors $A^iu_n, i = 0, 1, \ldots, k-1$, (6.6) reduces to

$$\beta_{ij} = (BH)_{i+1,j}, \qquad 0 \le i \le j;\ \beta_{0j} \equiv 0 \text{ all } j \ge 1. \tag{6.7}$$

Now $\beta_{11} = 1$ since $v_1 = u_n$. These equations can be solved in the order $i = 0, 1, \ldots, j, j = 1, 2, \ldots, k-1$, which amounts to computing the 1st, 2nd, $\ldots$, kth columns of the matrix B, in this order. This can be accomplished as $h_{j+1,j} > 0$ for all j. Thus by letting $i = 0$ in (6.7), we obtain $\sum_{r=1}^{j+1}\beta_{1r}h_{rj} = 0$, which we solve for $\beta_{1,j+1}$. Next, letting $i = 1$, we obtain $\beta_{1j} = \sum_{r=1}^{j+1}\beta_{2r}h_{rj}$, which we solve for $\beta_{2,j+1}$. By letting $i = 2, 3, \ldots, j$, we obtain $\beta_{i+1,j+1}, i = 2, 3, \ldots, j$, in this order.

Suppose that the Ritz vector $\hat{x}$ has been computed in the form $\hat{x} = \sum_{i=1}^{k}\xi_iv_i$ and that the ξ_i have been saved. Then, recalling also that $u_{n+i} = A^iu_n, i = 0, 1, \ldots, k-1$,

$$\hat{x} = \sum_{i=0}^{k-1}\sigma_iu_{n+i}, \tag{6.8}$$

and the coefficient of u_n is given by

$$\sigma_0 = \sum_{j=1}^{k}\beta_{1j}\xi_j. \tag{6.9}$$

Similarly, from (3.19), the coefficient of u_n in $\hat{d}_{ji,l}(n)$ (setting $\nu = -1$ there) is given by

$$\sigma_0' = (\hat{z} - \zeta_j(n))^i\frac{\sum_{r=1}^{k}c_r^{(n,k)}\hat{z}^{k-r}}{\sum_{r=0}^{k}c_r^{(n,k)}(k-r)\hat{z}^{k-r-1}} = -(\hat{z} - \zeta_j(n))^i\frac{c_0^{(n,k)}\hat{z}^k}{Q_{n,k}'(\hat{z})}. \tag{6.10}$$

Now if we denote the Ritz values by $\lambda'_1, \ldots, \lambda'_k$ and set $z'_i = 1/\lambda'_i, i = 1, \ldots, k$, then we can show that

$$\sigma'_0 = -(\hat{z} - \zeta_j(n))^i \frac{\hat{z}}{\prod_{\substack{r=1 \\ z'_r \neq \hat{z}}}^{k} (1 - z'_r/\hat{z})}, \tag{6.11}$$

so that

$$\hat{d}_{ji,l}(n) = \frac{\sigma'_0}{\sigma_0}\hat{x} = -\frac{(\hat{z} - \zeta_j(n))^i}{\prod_{\substack{r=1 \\ z'_r \neq \hat{z}}}^{k} (1 - z'_r/\hat{z})} \frac{\hat{z}}{\sum_{j=1}^{k} \beta_{1j}\xi_j}\hat{x}, \tag{6.12}$$

which is the desired result.

With this we can now go on to compute the approximations to the eigenvector a_{jp_j} and the vectors $a_{ji}, 0 \leq i < p_j - 1$, precisely as described in §§3.2.1 and 3.2.2, respectively. For example, the vector $\hat{d}_{jp_j}(n) = \sum_{l=1}^{\omega_j} \hat{d}_{jp_j,l}(n)$ is the approximation to the eigenvector a_{jp_j} the error in which is, roughly speaking, $O(|\lambda_{t+1}/\lambda_j|^n)$ as $n \to \infty$.

7. Numerical examples. In this section we demonstrate by numerical examples the validity of some of the theory and claims of the previous sections. The computations for this section were done in double precision arithmetic on an IBM-370 machine.

Example 7.1. Consider the 11×11 real symmetric matrix

$$A = 0.06 \times \begin{bmatrix} 5 & 2 & 1 & 1 & & & & & & & \\ 2 & 6 & 3 & 1 & 1 & & & & & & \\ 1 & 3 & 6 & 3 & 1 & 1 & & & & & \\ 1 & 1 & 3 & 6 & 3 & 1 & 1 & & & & \\ & 1 & 1 & 3 & 6 & 3 & 1 & 1 & & & \\ & & 1 & 1 & 3 & 6 & 3 & 1 & 1 & & \\ & & & 1 & 1 & 3 & 6 & 3 & 1 & 1 & \\ & & & & 1 & 1 & 3 & 6 & 3 & 1 & 1 \\ & & & & & 1 & 1 & 3 & 6 & 3 & 1 \\ & & & & & & 1 & 1 & 3 & 6 & 2 \\ & & & & & & & 1 & 1 & 2 & 5 \end{bmatrix}. \tag{7.1}$$

This matrix has 10 distinct positive eigenvalues, the smallest and largest being 0.0313 $\cdots$ and 0.896 $\cdots$, respectively. We applied the SMPE and SMMPE procedures to approximate its eigenvalues. With $u_0 = (1, 1, \ldots, 1)^T$, only 6 of the 10 eigenvalues appear in the spectral decomposition of u_m for all m. To five-digit accuracy these eigenvalues are $\lambda_1 = 0.89651, \lambda_2 = 0.52971, \lambda_3 = 0.26440, \lambda_4 = 0.24775, \lambda_5 = 0.19029$, and $\lambda_6 = 0.031337$.

In Tables 7.1.1 and 7.1.2 we give the errors $e_j(n) = \lambda_j - \lambda_j(n)$ in the approximations $\lambda_j(n), j = 1, 2, 3$, that were obtained by, respectively, the SMMPE and the SMPE procedures with $k = 3$. Here $\lambda_j(n)$ stands for $\lambda_{j1}(n)$, and we know that $\omega_j = 1$ for all j. Recall that for the SMPE procedure these $\lambda_j(n)$ are simply the Ritz values obtained by the Arnoldi method of order $k = 3$ as this method is being applied to u_n. They are also the Ritz values obtained by the Lanczos method of order $k = 3$ as this method is being applied to u_n with $q = u_n$ in (4.9). (The $\lambda_j(n)$ were actually obtained by solving the polynomial equation $\sum_{i=0}^{k} c_i^{(n,k)} \lambda^i = 0$ with

Table 7.1.1.
Errors in $\lambda_j(n)$ *obtained from* SMMPE *procedure with* $k = 3$ *on the matrix* A *in Example* 7.1. *The vector* u_0 *is* $(1, 1, \ldots, 1)^T$. *Here* $e_j(n) = \lambda_j - \lambda_j(n)$, $j = 1, 2, 3$.

n	$e_1(n)$	$e_2(n)$	$e_3(n)$
0	2.01D−02	1.15D−01	6.54D−02
1	5.02D−03	4.31D−02	3.78D−02
2	1.30D−03	1.82D−02	3.03D−02
3	3.38D−04	7.87D−03	2.61D−02
4	8.57D−05	3.39D−03	2.28D−02
5	2.15D−05	1.45D−03	2.00D−02
6	5.37D−06	6.21D−04	1.77D−02
7	1.35D−06	2.68D−04	1.58D−02
8	3.44D−07	1.17D−04	1.42D−02
9	8.84D−08	5.13D−05	1.29D−02
10	2.31D−08	2.29D−05	1.18D−02
11	6.10D−09	1.03D−05	1.09D−02
12	1.63D−09	4.72D−06	1.02D−02
13	4.42D−10	2.18D−06	9.54D−03
14	1.21D−10	1.01D−06	8.99D−03
15	3.32D−11	4.74D−07	8.52D−03

Table 7.1.2.
Errors in $\lambda_j(n)$ *obtained from* SMPE *procedure with* $k = 3$ *on the matrix* A *in Example* 7.1. *The vector* u_0 *is* $(1, 1, \ldots, 1)^T$. *Here* $e_j(n) = \lambda_j - \lambda_j(n)$, $j = 1, 2, 3$.

n	$e_1(n)$	$e_2(n)$	$e_3(n)$
0	7.01D−05	6.92D−03	2.26D−02
1	1.11D−06	3.64D−04	9.64D−03
2	5.43D−08	5.23D−05	6.84D−03
3	2.91D−09	8.15D−06	5.18D−03
4	1.65D−10	1.34D−06	4.11D−03
5	9.93D−12	2.36D−07	3.40D−03
6	6.41D−13	4.41D−08	2.88D−03
7	4.42D−14	8.73D−09	2.50D−03
8	3.62D−15	1.80D−09	2.18D−03
9	1.11D−15	3.81D−10	1.92D−03
10	6.25D−16	8.21D−11	1.70D−03

the $c_i^{(n,k)}$ determined from (1.6) and $c_k^{(n,k)} = 1$.) Note that the errors are all positive, and, for the SMPE procedure, this is consistent with the asymptotic result of [Si3, Thm. 2.1]. In addition, we have $e_j(n) = O(|\lambda_4/\lambda_j|^n)$ as $n \to \infty$ for SMMPE procedure (cf. (3.4)) and $e_j(n) = O(|\lambda_4/\lambda_j|^{2n})$ as $n \to \infty$ for SMPE procedure (cf. (3.11)). These can be verified numerically by computing $r_j(n) = e_j(n+1)/e_j(n)$, for which, $\lim_{n\to\infty} r_j(n) = \lambda_4/\lambda_j$ for SMMPE procedure and $\lim_{n\to\infty} r_j(n) = (\lambda_4/\lambda_j)^2$ for SMPE procedure. Indeed, $r_j(n)$ do approach their respective limits with increasing n.

The vectors $q_1, \ldots, q_k$ in the SMMPE procedure were taken to be the first k standard basis vectors for this example.

We should note, of course, that as n is increased, roundoff errors cause the vectors $u_n, u_{n+1}, \ldots$, to have contributions from *all* eigenvalues of A. With the precision we are using, at $n = 15$ the roundoff errors are still not sufficiently effective to cause this to happen in appreciable amounts.

Finally, if the above is repeated with $k = 4$, a significant improvement in the convergence rates of the $\lambda_j(n)$ is observed, as predicted by the theory of §3. This point has been explained in the third paragraph following the statement of Theorem 3.1.

Example 7.2. Consider the $m^2 \times m^2$ block tridiagonal matrix

$$A = \begin{bmatrix} B & -I & & \\ -I & B & -I & \\ & \ddots & \ddots & \ddots \\ & & & -I \\ & & -I & B \end{bmatrix}, \tag{7.2}$$

where I is the $m \times m$ identity matrix, B is the $m \times m$ real nonsymmetric tridiagonal matrix given by

$$B = \begin{bmatrix} 4 & a & & & \\ b & 4 & a & & \\ & \ddots & \ddots & \ddots & \\ & & b & 4 & a \\ & & & b & 4 \end{bmatrix}, \quad a = -1 + \frac{\gamma}{2(m+1)}, \quad b = -1 - \frac{\gamma}{2(m+1)}. \tag{7.3}$$

This matrix, with $\gamma = 1$, appears in [Sa1, Example 4.2.2], where it is treated with the help of the Arnoldi method when $m = 15$. It arises from central difference discretization of the elliptic operator $-(\partial^2/\partial x^2 + \partial^2/\partial y^2) + \gamma(\partial/\partial x)$ on the unit square with Dirichlet boundary conditions, the number of points of discretization interior to the unit square being m in each direction.

It can be shown that A is diagonalizable and that its eigenvalues are given by

$$\Lambda_{p,q}(\gamma) = 4 - 2\cos\frac{q\pi}{m+1} - 2\sqrt{1 - \left[\frac{\gamma}{2(m+1)}\right]^2}\cos\frac{p\pi}{m+1}, \quad p, q = 1, 2, \ldots, m. \tag{7.4}$$

To be able to compare our numerical results with those of [Sa1], we also applied the Arnoldi method to the matrix A with $\gamma = 1$ and $m = 15$. In this case all eigenvalues of A are real and positive. In Table 7.2.1 we give the errors in the Ritz values λ_1' and λ_2' that are approximations to the first two largest eigenvalues of A, namely, $\Lambda_{m,m}(1)$ and $\Lambda_{m-1,m}(1)$, for $k = 1, 2, \ldots$, obtained by applying the Arnoldi method of order k to a randomly generated vector u_0, as is commonly done. We also give the l_2-norms of the residuals $Ax_j' - \lambda_j' x_j', j = 1, 2$, where x_j' is the Ritz vector corresponding to λ_j', and $(x_j', x_j') = 1$. These norms are computed precisely in the way described in [Sa1, Eq. (3.14)]. In Tables 7.2.2 and 7.2.3 we do the same, except that we now apply the Arnoldi method to $u_n = A^n u_0$, with $n = 100$ and $n = 200$, respectively, u_0 being again a randomly generated vector.

Comparison of the results in Tables 7.2.1–7.2.3 shows first of all that the largest Ritz values converge much faster in k for $n = 100$ and $n = 200$ than for $n = 0$. Also the

TABLE 7.2.1.

Errors in the two largest Ritz values and l_2-norms of the residuals of corresponding Ritz vectors obtained from the Arnoldi method on the matrix A of Example 7.2 with $\gamma = 1$ and $m = 15$. The method is applied to the randomly generated vector u_0. Here $e_j^{(k)} = |\lambda_j - \lambda'_j|$ and $w_j^{(k)} = \|Ax'_j - \lambda'_j x'_j\|$, (λ'_j, x'_j) being pairs of Ritz values and Ritz vectors obtained from the Arnoldi method of order k, and $\|x'_j\| = 1$.

k	$e_1^{(k)}$	$w_1^{(k)}$	$e_2^{(k)}$	$w_2^{(k)}$
1	6.70D+00	1.89D+00		
2	2.54D+00	1.72D+00	7.44D+00	7.78D−01
3	1.19D+00	1.16D+00	4.55D+00	1.44D+00
4	6.56D−01	7.62D−01	3.03D+00	1.24D+00
5	3.88D−01	5.77D−01	2.02D+00	1.06D+00
6	2.44D−01	4.41D−01	1.40D+00	8.75D−01
7	1.62D−01	3.30D−01	1.03D+00	6.94D−01
8	1.16D−01	2.61D−01	7.82D−01	6.08D−01
9	8.34D−02	2.28D−01	5.78D−01	5.63D−01
10	5.85D−02	2.08D−01	4.13D−01	5.06D−01
11	4.10D−02	1.77D−01	3.04D−01	4.16D−01
12	2.74D−02	1.57D−01	2.24D−01	3.60D−01
13	1.86D−02	1.23D−01	1.74D−01	2.83D−01
14	1.31D−02	9.71D−02	1.40D−01	2.31D−01
15	9.18D−03	8.89D−02	1.12D−01	2.26D−01
16	6.71D−03	7.18D−02	8.98D−02	1.97D−01
17	4.37D−03	7.78D−02	6.34D−02	2.32D−01
18	2.42D−03	6.91D−02	3.77D−02	2.12D−01
19	1.22D−03	5.30D−02	2.08D−02	1.65D−01
20	5.72D−04	3.88D−02	1.11D−02	1.24D−01
21	2.28D−04	2.92D−02	5.32D−03	9.84D−02
22	1.00D−04	1.87D−02	2.74D−03	6.73D−02
23	5.02D−05	1.27D−02	1.42D−03	4.94D−02
24	2.86D−05	7.78D−03	7.01D−04	3.25D−02
25	1.85D−05	5.48D−03	3.02D−04	2.48D−02
26	1.16D−05	4.83D−03	1.53D−06	2.43D−02
27	7.95D−06	3.12D−03	1.63D−04	1.73D−02
28	6.46D−06	1.58D−03	2.15D−04	9.42D−03
29	5.60D−06	9.05D−04	2.19D−04	5.73D−03
30	4.80D−06	5.57D−04	2.06D−04	3.75D−03

cost, both storagewise and computational, of obtaining a high level accuracy is larger when $n = 0$ than when $n > 0$ and is sufficiently large. For instance, the accuracy attained for λ'_1 with $n = 0$ and $k = 30$ can be attained with $n = 100$ and $k = 5$. In the former we must store 30 vectors, whereas in the latter we need to store 5 vectors. Roughly speaking, the computational effort in the former case is the equivalent of about 232 matrix-vector products, whereas in the latter this number is 144.

We determine computational cost in the following way. First of all, if we are interested only in the eigenvalues, then the computational cost is the sum of (i) the n matrix-vector products to get to u_n along with the n normalizations for $u_0, u_1, \ldots, u_{n-1}$, cf. (6.1), and (ii) the cost of forming the matrix V_{k-1}, cf. (4.6). The cost of (i) is n matrix-vector products, n scalar products, and n scalar-vector multiplications. The cost of (ii) is $k-1$ matrix-vector products, $\frac{1}{2}k(k+1)$ scalar products, $\frac{1}{2}k(k+1)$

TABLE 7.2.2.

Errors in the two largest Ritz values and l_2-norms of the residuals of corresponding Ritz vectors obtained from the Arnoldi method on the matrix A of Example 7.2 with $\gamma = 1$ and $m = 15$. The method is applied to the vector $u_n = A^n u_0$ with $n = 100$, where u_0 is a randomly generated vector. Here $e_j^{(k)} = |\lambda_j - \lambda'_j|$ and $w_j^{(k)} = \|Ax'_j - \lambda'_j x'_j\|, (\lambda'_j, x'_j)$ being pairs of Ritz values and Ritz vectors obtained from the Arnoldi method of order k, and $\|x'_j\| = 1$.

k	$e_1^{(k)}$	$w_1^{(k)}$	$e_2^{(k)}$	$w_2^{(k)}$
1	1.46D−02	4.98D−02		
2	1.58D−03	1.97D−02	1.65D−02	7.12D−02
3	8.74D−06	5.19D−03	1.56D−05	2.59D−02
4	2.14D−06	6.15D−04	1.33D−04	4.26D−03
5	2.79D−06	9.87D−05	1.61D−04	8.65D−04
6	2.33D−06	3.64D−05	1.17D−04	4.66D−04
7	4.30D−07	1.62D−05	2.45D−05	3.12D−04
8	1.29D−06	3.19D−06	1.86D−05	7.40D−05
9	8.28D−06	1.02D−06	6.39D−05	2.78D−05
10	1.60D−06	7.35D−08	2.19D−05	2.06D−06
11	9.04D−09	1.64D−07	7.99D−06	5.23D−06
12	2.09D−07	5.17D−08	1.02D−05	1.85D−06
13	2.56D−09	5.06D−08	7.76D−06	2.48D−06
14	1.16D−07	5.36D−08	1.04D−05	3.96D−06
15	1.88D−08	4.49D−08	5.33D−06	1.22D−05
16	2.14D−08	1.28D−08	9.42D−06	5.25D−06
17	1.10D−08	2.01D−08	9.72D−08	3.00D−05
18	3.90D−09	5.96D−09	7.69D−06	2.06D−05
19	3.93D−09	6.15D−09	1.42D−05	6.70D−05
20	8.85D−10	2.74D−09	1.09D−05	2.05D−04

scalar-vector multiplications, and $\frac{1}{2}k(k-1)$ vector additions. If we agree to consider a scalar product as consisting of a scalar-vector multiplication and a vector addition, the total number of operations will be $n + k - 1$ matrix-vector products, $2n + k^2 + k$ scalar-vector multiplications, and $n + k^2$ vector additions. Finally, let us make the simplification that addition and multiplication have the same cost. All this, of course, is not most accurate, but gives a reasonable account of the cost. In our example, one matrix-vector product is very nearly equivalent to five scalar-vector multiplications and four vector additions.

The approximation λ'_1 that corresponds to $n = 100$ and $k = 20$ in Table 7.2.2 has about the same accuracy as that given in [Sa1]. But the way the approximation of [Sa1] is obtained is much more complicated and also more expensive computationally.

Now with $\gamma = 1$, the matrix A is close to being symmetric, and one may attribute the good results shown in Tables 7.2.2 and 7.2.3 to this fact. We, therefore, applied the Arnoldi method with larger values of γ that cause A to become highly nonsymmetric. Our results and conclusions were invariably the same. Actually, when the Arnoldi method was applied with large values of γ, e.g., $\gamma = 10$, the quality of the Ritz values with $n = 0$ deteriorated, whereas the quality of those with $n = 100$ remained almost the same.

Finally, we have also applied the Arnoldi method to $M = I - \frac{1}{4}A$ with $\gamma = 0$.

TABLE 7.2.3.

Errors in the two largest Ritz values and l_2-norms of the residuals of corresponding Ritz vectors obtained from the Arnoldi method on the matrix A of Example 7.2 with $\gamma = 1$ and $m = 15$. The method is applied to the vector $u_n = A^n u_0$ with $n = 200$, where u_0 is a randomly generated vector. Here $e_j^{(k)} = |\lambda_j - \lambda'_j|$ and $w_j^{(k)} = \|Ax'_j - \lambda'_j x'_j\|$, (λ'_j, x'_j) being pairs of Ritz values and Ritz vectors obtained from the Arnoldi method of order k, and $\|x'_j\| = 1$.

k	$e_1^{(k)}$	$w_1^{(k)}$	$e_2^{(k)}$	$w_2^{(k)}$
1	5.61D−02	5.76D−02		
2	8.43D−05	4.08D−02	7.03D−05	8.33D−03
3	3.57D−06	1.61D−03	7.28D−05	5.34D−04
4	6.00D−07	1.15D−04	2.49D−05	6.79D−05
5	2.10D−07	2.48D−05	5.51D−05	2.24D−05
6	1.56D−07	1.01D−06	5.53D−05	1.14D−06
7	5.25D−07	2.53D−07	4.72D−05	7.12D−07
8	5.23D−07	1.56D−08	6.31D−05	5.12D−08
9	1.03D−08	8.23D−08	5.09D−05	6.30D−06
10	1.03D−08	4.88D−09	6.12D−05	6.02D−07
11	2.86D−09	8.36D−09	2.13D−05	2.02D−05
12	3.58D−10	1.08D−09	2.96D−05	1.28D−05
13	2.56D−10	3.96D−10	3.47D−06	1.31D−05
14	1.96D−10	6.09D−10	5.71D−06	2.25D−05
15	4.51D−11	1.94D−10	1.98D−06	1.01D−05
16	1.94D−11	5.69D−11	7.79D−07	3.21D−06
17	1.99D−11	6.86D−11	1.65D−06	4.12D−06
18	1.01D−11	5.74D−11	6.09D−07	4.05D−06
19	5.32D−12	2.48D−11	8.41D−07	1.87D−06
20	4.67D−12	2.84D−11	2.44D−07	2.44D−06

This matrix is real symmetric and its spectrum is in $(-1, 1)$ and is symmetric with respect to the origin. Again the results obtained from the Arnoldi (now equivalent to symmetric Lanczos) method with $n > 0$ and large were superior to those obtained with $n = 0$.

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