

FEAST AS A SUBSPACE ITERATION EIGENSOLVER ACCELERATED BY APPROXIMATE SPECTRAL PROJECTION*

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Abstract. The calculation of a segment of eigenvalues and their corresponding eigenvectors of a Hermitian matrix or matrix pencil has many applications. A new density-matrix-based algorithm has been proposed recently and a software package FEAST has been developed. The density-matrix approach allows FEAST's implementation to exploit a key strength of modern computer architectures, namely, multiple levels of parallelism. Consequently, the software package has been well received, especially in the electronic structure community. Nevertheless, theoretical analysis of FEAST has lagged. For instance, the FEAST algorithm has not been proven to converge. This paper offers a detailed numerical analysis of FEAST. In particular, we show that the FEAST algorithm can be understood as an accelerated subspace iteration algorithm in conjunction with the Rayleigh–Ritz procedure. The novelty of FEAST lies in its accelerator, which is a rational matrix function that approximates the spectral projector onto the eigenspace in question. Analysis of the numerical nature of this approximate spectral projector and the resulting subspaces generated in the FEAST algorithm establishes the algorithm's convergence. This paper shows that FEAST is resilient against rounding errors and establishes properties that can be leveraged to enhance the algorithm's robustness. Finally, we propose an extension of FEAST to handle non-Hermitian problems and suggest some future research directions.

Key words. generalized eigenvalue problem, subspace iteration, spectral projection

AMS subject classifications. 15A18, 65F15

DOI. 10.1137/13090866X

1. Introduction. Solving matrix eigenvalue problems is crucial in many scientific and engineering applications. Robust solvers for problems of moderate size are well developed and widely available [2]. These are sometimes referred to as direct solvers [6]. Direct solvers typically calculate the entire spectrum of the matrix or matrix pencil in question. Yet in many applications, especially those where the underlying linear systems are large and sparse, it is often the case that only selected segments of the spectrum are of interest. Polizzi recently proposed a density-matrix-based algorithm [21] named FEAST for Hermitian eigenproblems of this kind. From an implementation point of view, FEAST's main building block is a numerical-quadrature computation consisting of solving independent linear systems, each for multiple right-hand sides. This building block contains multiple levels of parallelism and thus exploits the features of modern computing architectures very well. A software package FEAST [22] based on this approach has been made available since 2009. Nevertheless, theoretical analysis of FEAST has been lagging. In particular, there is no theoretical study available on the conditions under which FEAST converges, and if so, at what rate.

This paper shows that the FEAST algorithm can be understood as a standard subspace iteration in conjunction with the Rayleigh–Ritz procedure. FEAST, therefore, belongs to the class of projection methods that typically construct bases

*Received by the editors February 5, 2013; accepted for publication (in revised form) by V. Simoncini January 7, 2014; published electronically April 3, 2014.

<http://www.siam.org/journals/simax/35-2/90866.html>

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to particular subspaces and then obtain the corresponding Ritz values and vectors (e.g., see [25, Chapter 6]). In Krylov projection methods such as Lanczos [3, 5, 20] or Arnoldi [17], the subspace at iteration m is spanned by a set of the form $\{\mathbf{v}, M\mathbf{v}, M^2\mathbf{v}, \dots, M^{m-1}\mathbf{v}\}$, where M is the matrix in question. The dimensions of the subspaces grow as iterations proceed. The initial vector \mathbf{v} can be chosen at random, or constructed carefully including the use of a “filter” $\mathbf{v} = \rho(M)\mathbf{v}_0$ for some \mathbf{v}_0 . Filters are often called accelerators because they can hasten convergence when chosen appropriately. We use the two terms interchangeably throughout this paper. Very often, the accelerator $\rho(M)$ is a polynomial in M [24, 35]. Jacobi–Davidson [29] is another notable projection method on expanding subspaces. More recently, Sakurai and Sugiura [26] proposed a projection method (SS-projection) that uses certain moment matrices. SS-projection is subsequently recognized as a Krylov method in [13] (see Theorem 7) and generalized to a block Krylov method [13, 12]. In the terminology of filtered Krylov methods, the subspaces in SS-projection are spanned by sets of the form $\{\mathbf{v}, f(M)\mathbf{v}, f^2(M)\mathbf{v}, \dots, f^{m-1}(M)\mathbf{v}\}$, where \mathbf{v} is a filtered random vector $\mathbf{v} = \rho_0(M)\mathbf{v}_0$. Here \mathbf{v}_0 is chosen randomly, $\rho_0(M)$ approximates a zeroth-moment matrix, and $f^k(M)$, $k \geq 1$, approximates a k th moment matrix.

In contrast to these methods that project onto expanding subspaces, there is a class of projection methods that project onto subspaces of a fixed dimension. The subspaces, but not their dimensions, change as iterations proceed. Trace minimization [28, 27] is one example of such methods, but the classical representative is subspace iterations (see [4] or discussions in standard textbooks such as [3, 7, 6, 25]). Here the p -dimensional subspaces are spanned by vectors of the form $M^k V$, where V consists of p vectors chosen randomly. Accelerators (filters) can be applied so that the subspaces are spanned instead by vectors of the form $f_m(M) \cdot f_{m-1}(M) \cdots f_1(M)V$. The accelerators $f_k(M)$ can be the same for all k , or can be made adaptive to exploit new information gained as iterations proceed. In this context, we show that FEAST is a subspace iteration accelerated by a nonadaptive accelerator $f_k(M) = \rho(M)$ for all k , where $\rho(M)$ approximates the spectral projector to the invariant eigenspace in question. This accelerator $\rho(M)$, in fact, corresponds to the approximate zeroth-moment matrix $\rho_0(M)$ in the SS-projection method. Both filters are constructed in a similar way, exploiting the Cauchy integral formula. Nevertheless, as mentioned previously, SS-projection is fundamentally a Krylov method that uses subspaces spanned by sets of the form $\{\mathbf{v}, f(M)\mathbf{v}, f^2(M)\mathbf{v}, \dots, f^{m-1}(M)\mathbf{v}\}$, \mathbf{v} being a filtered starting vector: $\mathbf{v} = \rho_0(M)\mathbf{v}_0$ for some randomly chosen \mathbf{v}_0 . The matrices $f^k(M)$, $k \geq 1$, approximate the k th moment matrices. In contrast, FEAST is fundamentally a subspace iteration eigensolver. It uses subspaces spanned by sets of the form $\rho^k(M)V$. Note that $\rho^k(M)$ does not approximate the k th moment matrix at all, but rather approximates the spectral projector progressively better as k advances.

Standard theory in the literature readily establishes FEAST’s convergence whenever we identify it as an accelerated subspace iteration. Nevertheless, to fully understand the algorithm’s fast convergence and possible modes of failure, detailed analysis specific to the use of FEAST’s accelerator is carried out in this paper. Furthermore, this analysis allows us to improve the robustness of the original algorithm that was proposed in [21]. The resulting enhancements include estimation of the number of eigenvalues in the segment of interest, and evaluation of whether the dimension chosen for the subspaces is appropriate. This paper puts FEAST on a more solid foundation. Finally, we outline at the end of this paper how FEAST can be extended to handle non-Hermitian problems.

2. Overview. Throughout this paper, we consider two $n \times n$ Hermitian matrices A and B , where B is positive definite; that is, $B = C^*C$ for some invertible matrix C , where C^* denotes the complex-conjugate transposition of C . We state some well-known properties germane to our presentation. There exists an $n \times n$ B -orthogonal matrix X , $X^*BX = I$, such that $AX = BX\Lambda$, where Λ is a real diagonal matrix. Each diagonal entry λ of Λ , together with its corresponding vector \mathbf{x} of X , constitute an eigenpair (λ, \mathbf{x}) : $A\mathbf{x} = \lambda B\mathbf{x} \iff (B^{-1}A)\mathbf{x} = \lambda\mathbf{x}$. Determining eigenpairs for the generalized problem given by (A, B) is equivalent to determining eigenpairs for the single matrix $B^{-1}A$. Moreover, $X^*BX = I$ implies $X^{-1} = X^*B$ and

$$(2.1) \quad M \stackrel{\text{def}}{=} B^{-1}A = X\Lambda X^{-1} = X\Lambda X^*B.$$

This paper focuses on the following problem. Given an interval $\mathcal{I} = [\lambda_-, \lambda_+]$ on the real line, determine (counting multiplicities) all e eigenpairs (λ, \mathbf{x}) , $M\mathbf{x} = \lambda\mathbf{x}$, where $\lambda \in \mathcal{I}$.

The following is a simple variant of Algorithms 5.3 and 7.5 in [25]. It is a subspace iteration algorithm with projection that also uses an accelerator $\rho(M)$.

Algorithm A. Accelerated subspace iteration with Rayleigh–Ritz

- 1: Pick p random n -vectors $Q_{(0)} = [\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_p]$. Set $k \leftarrow 1$.
 - 2: **repeat**
 - 3: Approximate subspace projection: $Y_{(k)} \leftarrow \rho(M) \cdot Q_{(k-1)}$.
 - 4: Form reduced system: $\hat{A}_{(k)} \leftarrow Y_{(k)}^* A Y_{(k)}$, $\hat{B}_{(k)} \leftarrow Y_{(k)}^* B Y_{(k)}$.
 - 5: Solve p -dimension eigenproblem: $\hat{A}_{(k)} \hat{X}_{(k)} = \hat{B}_{(k)} \hat{X}_{(k)} \hat{\Lambda}_{(k)}$ for $\hat{\Lambda}_{(k)}$, $\hat{X}_{(k)}$.
 - 6: Set $Q_{(k)} \leftarrow Y_{(k)} \hat{X}_{(k)}$; in particular, $Q_{(k)}^* B Q_{(k)} = I_p$.
 - 7: $k \leftarrow k + 1$.
 - 8: **until** Appropriate stopping criteria
-

Without acceleration, that is, when $\rho(M) = M$, Algorithm A corresponds simply to straightforward subspace iteration with the Rayleigh–Ritz procedure. If we denote by $X_{\mathcal{I}}$ the set of columns from X corresponding to the eigenvectors of interest, then the choice $\rho(M) = X_{\mathcal{I}} X_{\mathcal{I}}^* B$, the spectral projector to the invariant subspace spanned by $X_{\mathcal{I}}$, is an ideal accelerator. Algorithm A converges in one iteration if p is chosen to be e and $Y_{(1)} = \rho(M)Q_{(0)}$ happens to have full rank. The reason is that, under these assumptions, $Y_{(1)} = X_{\mathcal{I}} W^{-1}$ for some invertible $W \in \mathbb{C}^{e \times e}$. This leads to

$$\hat{A}_{(1)} = (W^{-1})^* \Lambda_{\mathcal{I}} W^{-1} \quad \text{and} \quad \hat{B}_{(1)} = (W^{-1})^* W^{-1},$$

where $\Lambda_{\mathcal{I}}$ is a diagonal matrix whose diagonal entries are exactly the eigenvalues of interest, $\lambda \in \mathcal{I}$, counting multiplicities. One can show that the Ritz values and vectors are indeed the eigenpairs of interest.

While the (exact) spectral projector $X_{\mathcal{I}} X_{\mathcal{I}}^* B$ is not readily available, it turns out that $\rho(M)$ approximates it quite well when $\rho(\mu)$ is a rational function constructed via a Gauss–Legendre quadrature. With this accelerator, Algorithm A is exactly the FEAST algorithm as stated in [21].

In the following sections, we analyze FEAST’s convergence behavior.

- Section 3 constructs a rational function $\rho : \mathbb{C} \rightarrow \mathbb{C}$ for a specified $\mathcal{I} = [\lambda_-, \lambda_+]$. The properties of the function $\rho(\mu)$ for μ restricted on the real line are studied. These properties explain why and in what sense the matrix function $\rho(M)$ approximates a spectral projector.

- Section 4 establishes that the distances from an eigenvector of interest to $\text{span}(Q_{(k)})$ converge to zero, where $Q_{(k)}$ is generated according to Algorithm A. The first theorem there is a straightforward generalization of Theorem 5.2 from [25], taking into account (1) the special properties of $\rho(M)$, and (2) that we are dealing with a generalized eigenvalue problem. The second theorem examines the impact on convergence when the application of $\rho(M)$ to vectors, and, in particular, to the $Q_{(k)}$ s, contains errors. This study is relevant because, unlike polynomial accelerators, application of $\rho(M)$ involves solutions of linear systems (see section 3 for details).
- The Rayleigh–Ritz procedure is needed to derive the actual desired eigenpairs from merely a basis $Q_{(k)}$ of the subspace $\mathcal{Q}_{(k)} = \text{span}(Q_{(k)})$ that is close to the desired eigenvectors. Section 5 analyzes the convergence properties of eigenpairs, taking into account the idiosyncrasies of $\mathcal{Q}_{(k)}$ due to the use of $\rho(M)$ as an accelerator. Some of the consequences of these idiosyncrasies were, in fact, observed in [15], and now have a satisfactory explanation. We also show that eigenvalues of $\widehat{B}_{(k)}$ offer accurate estimates of e , the number of eigenvalues inside \mathcal{I} . These properties can be exploited in an enhanced version of FEAST.
- Section 6 presents a number of computational examples to illustrate key aspects of the preceding analysis as well as numerical subtleties.

3. Approximate spectral projector $\rho(M)$. Given an interval $\mathcal{I} = [\lambda_-, \lambda_+]$ on the real line, $\lambda_- < \lambda_+$, we will construct a rational function $\rho : \mathbb{C} \rightarrow \mathbb{C}$ such that $\rho(\mu) \in \mathbb{R}$ for $\mu \in \mathbb{R}$, and such that the function $\rho(\mu)$ restricted on the real line is a good approximation to the indicator function of \mathcal{I} . To accomplish this, we use a Cauchy integral representation of the indicator function and construct $\rho(\mu)$ based on a numerical quadrature rule.

3.1. Construction of $\rho(\mu)$. Let \mathcal{C} be the circle centered at $c = (\lambda_+ + \lambda_-)/2$ with radius $r = (\lambda_+ - \lambda_-)/2$. Define the function $\pi(\lambda)$ by the contour integral (in the counterclockwise direction)

$$(3.1) \quad \pi(\mu) = \frac{1}{2\pi i} \oint_{\mathcal{C}} \frac{1}{z - \mu} dz, \quad \mu \notin \mathcal{C}.$$

The Cauchy integral theorem shows that $\pi(\mu) = 1$ for $|\mu - c| < r$ and $\pi(\mu) = 0$ for $|\mu - c| > r$. We use a numerical quadrature to approximate the integral in (3.1). To this end, we define the parametrization $\phi(t)$, $-1 \leq t \leq 3$:

$$(3.2) \quad \phi(t) = c + r e^{i\frac{\pi}{2}(1+t)} \quad \text{and} \quad \phi'(t) = i\frac{\pi}{2} r e^{i\frac{\pi}{2}(1+t)}.$$

Thus,

$$(3.3) \quad \begin{aligned} \pi(\mu) &= \frac{1}{2\pi i} \int_{-1}^3 \frac{\phi'(t)}{\phi(t) - \mu} dt \\ &= \frac{1}{2\pi i} \left[\int_{-1}^1 \frac{\phi'(t)}{\phi(t) - \mu} dt + \int_{-1}^1 \frac{\phi'(2-t)}{\phi(2-t) - \mu} dt \right] \\ &= \frac{1}{2\pi i} \int_{-1}^1 \left[\frac{\phi'(t)}{\phi(t) - \mu} - \frac{\overline{\phi'(t)}}{\overline{\phi(t)} - \mu} \right] dt. \end{aligned}$$

We restrict ourselves to Gauss–Legendre quadratures on $[-1, 1]$ (see, for example, [32]). A q -point Gauss–Legendre quadrature rule is defined by a set of weight-node pairs

(w_k, t_k) , $k = 1, 2, \dots, q$, where $w_k > 0$ and $-1 < t_k < 1$. The set is symmetric in that both (w_k, t_k) and $(w_k, -t_k)$ are present. The choice of the weight-node pairs are meant to make $\sum_{k=1}^q w_k f(t_k)$ approximate $\int_{-1}^1 f(t) dt$ well for continuous function $f : [-1, 1] \rightarrow \mathbb{C}$. Moreover, for any polynomial f of degree at most $2q - 1$, the q -term summation produces the exact integral. In particular, $\sum_{k=1}^q w_k = 2$ (by taking $f \equiv 1$).

In a typical setting, a quadrature aims at producing a single value that approximates a specific definite integral of an integrand. Here, it corresponds to approximating $\pi(\mu)$ for a specific fixed μ . But if we use the same quadrature rule for all possible μ , we have, in fact, defined a function of μ . This is how we define our $\rho(\mu)$. Let (w_k, t_k) , $k = 1, 2, \dots, q$, be the q -point Gauss–Legendre rule of choice. We define the function $\rho(\mu)$ by the quadrature formula applied to the integral of (3.3):

$$(3.4) \quad \rho(\mu) \stackrel{\text{def}}{=} \frac{1}{2\pi i} \sum_{k=1}^q \left(\frac{w_k \phi'(t_k)}{\phi(t_k) - \mu} - \frac{w_k \overline{\phi'(t_k)}}{\overline{\phi(t_k)} - \mu} \right) = \sum_{k=1}^q \left(\frac{\sigma_k}{\phi_k - \mu} + \frac{\overline{\sigma_k}}{\overline{\phi_k} - \mu} \right),$$

$\phi_k = \phi(t_k)$, and $\sigma_k = w_k \phi'(t_k)/(2\pi i)$. Note that $\rho : \mathbb{C} \rightarrow \mathbb{C}$ is a rational function in partial fraction form. The $2q$ poles of $\rho(\mu)$ are ϕ_k and $\overline{\phi_k}$ for $k = 1, 2, \dots, q$. Because $-1 < t_k < 1$, these poles are all complex valued. Consequently, $\rho(\mu)$ is defined for all $\mu \in \mathbb{R}$. From (3.4), $\rho(\mu) = \overline{\rho(\mu)}$ for $\mu \in \mathbb{R}$. Thus $\rho(\mu) \in \mathbb{R}$ for $\mu \in \mathbb{R}$.

3.2. Computing $\rho(M)Q$. Consider our matrix $M = B^{-1}A$ and a function $f(x) = \alpha/(\beta - x)$, where α and β are constants, and $\beta I - M$ is invertible. It is common to define the function f of M , $f(M)$, as the matrix $\alpha(\beta I - M)^{-1}$ (see page 1 of [10]). Since M is diagonalizable, $M = X \Lambda X^{-1}$,

$$(3.5) \quad \begin{aligned} f(M) &\stackrel{\text{def}}{=} \alpha(\beta I - M)^{-1} \\ &= \alpha(\beta X X^{-1} - X \Lambda X^{-1})^{-1} \\ &= \alpha X (\beta I - \Lambda)^{-1} X^{-1} \\ (3.6) \quad &= X f(\Lambda) X^{-1}, \end{aligned}$$

where $f(\Lambda)$ is the standard definition of a function of a diagonal matrix: namely, replacing each diagonal entry λ of Λ with $f(\lambda)$. Clearly, for each eigenpair (λ, \mathbf{x}) of M , $(f(\lambda), \mathbf{x})$ is an eigenpair of $f(M)$.

As none of the ϕ_k s are on the real line while M 's eigenvalues are all real, $\phi_k I - M$, $\overline{\phi_k} I - M$, $k = 1, 2, \dots, q$, are all invertible. Following (3.5), we have

$$\begin{aligned} \rho(M) &= \sum_{k=1}^q \sigma_k (\phi_k I - M)^{-1} + \sum_{k=1}^q \overline{\sigma_k} (\overline{\phi_k} I - M)^{-1} \\ &= \sum_{k=1}^q \sigma_k (\phi_k B - A)^{-1} B + \sum_{k=1}^q \overline{\sigma_k} (\overline{\phi_k} B - A)^{-1} B. \end{aligned}$$

Therefore, for any $Q \in \mathbb{C}^{n \times p}$,

$$(3.7) \quad \begin{aligned} \rho(M)Q &= \sum_{k=1}^q \sigma_k (\phi_k B - A)^{-1} BQ + \sum_{k=1}^q \overline{\sigma_k} (\overline{\phi_k} B - A)^{-1} BQ \quad \text{in general,} \\ &= 2 \sum_{k=1}^q \text{Re} \left(\sigma_k (\phi_k B - A)^{-1} BQ \right) \quad \text{if } A, B, \text{ and } Q \text{ are real valued.} \end{aligned}$$

Application of $\rho(M)$ to Q involves, in general, solutions of $2q$ linear systems of equations with p right-hand sides each, but q linear systems only if A , B , and Q are all real matrices.

Substituting ρ for f in (3.6) gives

$$(3.8) \quad \rho(M) = X\rho(\Lambda)X^{-1} = X\rho(\Lambda)X^*B$$

because $M = X\Lambda X^{-1} = X\Lambda X^*B$. This implies that $(\rho(\lambda), \mathbf{x})$ is an eigenpair of $\rho(M)$ for any eigenpair (λ, \mathbf{x}) of M . Suppose $\rho(\lambda) = 1$ for all the e eigenvalues λ of M that lie inside $\mathcal{I} = [\lambda_-, \lambda_+]$ and $\rho(\lambda) = 0$ for all those $n - e$ that lie outside; then $\rho(M)$ is, in fact, the exact spectral projector $X_{\mathcal{I}}X_{\mathcal{I}}^*B$. In general, for any n -vector \mathbf{q} ,

$$(3.9) \quad \mathbf{q} = \sum_{\lambda \in \text{eig}(M)} \alpha_{\lambda} \mathbf{x}_{\lambda} \implies \rho(M)\mathbf{q} = \sum_{\lambda \in \text{eig}(M)} \alpha_{\lambda} \rho(\lambda) \mathbf{x}_{\lambda}.$$

Suppose the scalar function $\rho(\mu)$ approximates the indicator function well in the sense that $\rho(\lambda) \approx 1$ for eigenvalues λ inside \mathcal{I} and $|\rho(\lambda)| \ll 1$ for those eigenvalues λ outside of \mathcal{I} . Then $\rho(M)$ approximates the behavior of the exact projector $X_{\mathcal{I}}X_{\mathcal{I}}^*B$: $\rho(M)\mathbf{q}$ leaves almost invariant the component of \mathbf{q} in $\text{span}(X_{\mathcal{I}})$ while almost annihilating the component of \mathbf{q} in the complementary eigenspace. We will now study more closely how well $\rho(\mu)$ approximates the indicator function.

3.3. Properties of $\rho(\mu)$ and $\rho(M)$. As the spectrum of M is real and $\rho(M) = X\rho(\Lambda)X^{-1}$, it suffices to study $\rho(\mu)$ for $\mu \in \mathbb{R}$. As noted previously, $\rho(\mu) \in \mathbb{R}$ for $\mu \in \mathbb{R}$. Moreover, it suffices to study the reference function $\rho_{\text{ref}}(\mu)$ that corresponds to the interval $[-1, 1]$. This is because a general $\rho(\mu)$ that corresponds to $\mathcal{I} = [\lambda_-, \lambda_+]$ with center c and radius r is given by the simple relationship $\rho(\mu) = \rho_{\text{ref}}((\mu - c)/r)$ due to our choice of parametrization (3.2). Equation (3.4) shows that for $\mu \in \mathbb{R}$,

$$(3.10) \quad \begin{aligned} \rho_{\text{ref}}(\mu) &= \frac{1}{2} \sum_{k=1}^q w_k \operatorname{Re} \left(\frac{\phi_k}{\phi_k - \mu} \right) \\ &= \frac{1}{2} \sum_{k=1}^q w_k \frac{1 + \mu s_k}{1 + 2\mu s_k + \mu^2}, \quad s_k = \sin(\pi t_k/2). \end{aligned}$$

As noted previously, for each weight-node pair (w_k, t_k) , where $t_k > 0$, there is a pair $(w_{k'}, t_{k'})$, where $w_{k'} = w_k$ and $t_{k'} = -t_k$. Note also that $s_k = \sin(\pi t_k/2)$, and thus summing the pair

$$w_k \frac{1 + \mu s_k}{1 + 2\mu s_k + \mu^2} + w_{k'} \frac{1 + \mu s_{k'}}{1 + 2\mu s_{k'} + \mu^2} = w_k \left(\frac{1 + \mu s_k}{1 + 2\mu s_k + \mu^2} + \frac{1 - \mu s_k}{1 - 2\mu s_k + \mu^2} \right)$$

yields an even function. For $t_k = s_k = 0$,

$$w_k \frac{1 + \mu s_k}{1 + 2\mu s_k + \mu^2} = \frac{w_k}{1 + \mu^2}$$

is also an even function. As a result, $\rho_{\text{ref}}(\mu)$ is an even function. It suffices to study $\rho_{\text{ref}}(\mu)$ for $\mu \geq 0$.

Before we present proofs on several properties of $\rho_{\text{ref}}(\mu)$, let us examine some illustrative figures. Figure 1 suggests that for a reference interval $\mathcal{I} = [-1, 1]$ and the quadrature rule choice of $q = 8$, eigencomponents that correspond to eigenvalues $|\lambda| \geq 1.6$ will be attenuated by roughly four or more orders of magnitudes. Figure 1 also suggests that $\rho_{\text{ref}}(\mu) \geq 1/2$ for $\mu \in \mathcal{I}$ while $|\rho_{\text{ref}}(\mu)| \leq 1/2$ for $|\mu| \geq 1$. Figure 2 illustrates the attenuation properties of six specific Gauss–Legendre quadrature rules.

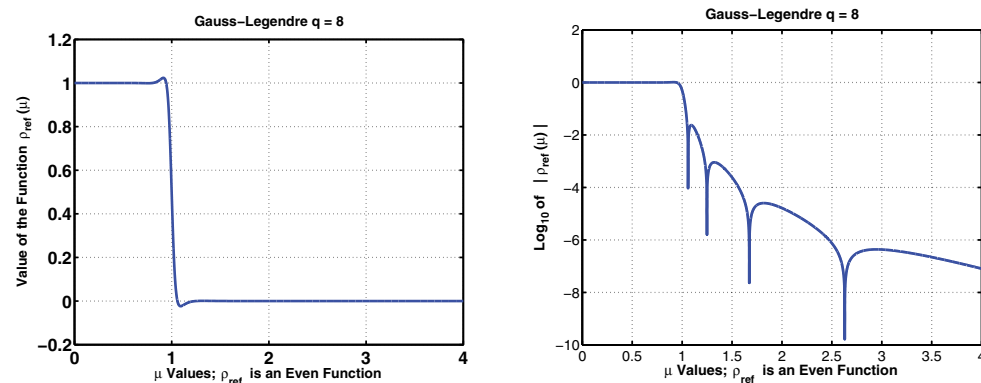


FIG. 1. An ideal $\rho_{\text{ref}}(\mu)$ function is 1 on $[-1, 1]$ and 0 elsewhere. This figure shows that $\rho_{\text{ref}}(\mu)$ obtained by Gauss-Legendre approximates this ideal well. We do not show $\rho_{\text{ref}}(\mu)$ for $\mu < 0$ because $\rho_{\text{ref}}(-\mu) = \rho_{\text{ref}}(\mu)$. The left picture shows the general shape of the function, while the logarithmic scale on the right illustrates how $|\rho_{\text{ref}}(\mu)|$ gets very small very soon beyond the reference $[\lambda_-, \lambda_+]$ of $[-1, 1]$.

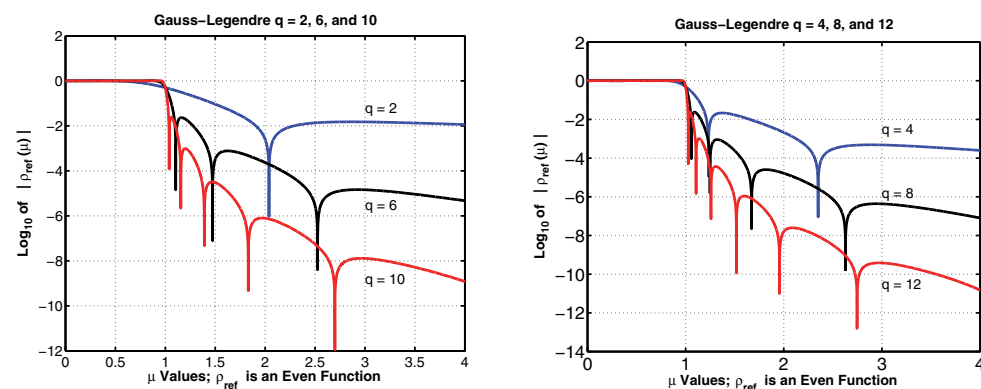


FIG. 2. This figure illustrates the decay properties of $|\rho_{\text{ref}}(\mu)|$ of different degrees q of Gauss-Legendre quadratures. The Y-axes are in logarithmic scale.

THEOREM 3.1. For a Gauss-Legendre quadrature of any choice $q \geq 1$, and the parametrization $\phi(t) = e^{-t\frac{\pi}{2}(1+t)}$, the following hold:

- (1) $\rho_{\text{ref}}(0) = 1$ and $\rho_{\text{ref}}(1) = 1/2$.
- (2) $\rho'_{\text{ref}}(1) < 0$.
- (3) $\rho_{\text{ref}}(\mu) \geq 1/2$ for $\mu \in [-1, 1]$.

Proof. Let (w_k, t_k) , $k = 1, 2, \dots, q$, be the weight-node pairs. Recall from (3.10) that

$$\rho_{\text{ref}}(\mu) = \frac{1}{2} \sum_{k=1}^q w_k \frac{1 + \mu s_k}{1 + 2\mu s_k + \mu^2}, \quad s_k = \sin(\pi t_k/2).$$

As noted before, $\sum_{k=1}^q w_k = 2$. Thus

$$\rho_{\text{ref}}(0) = \frac{1}{2} \sum_{k=1}^q w_k = 1 \quad \text{and} \quad \rho_{\text{ref}}(1) = \frac{1}{2} \sum_{k=1}^q w_k \frac{1}{2} = \frac{1}{2}.$$

This establishes (1).

Next, note that $-1 < t_k < 1$ implies $-1 < s_k < 1$ and $1 - s_k^2 > 0$. Thus,

$$\begin{aligned}\rho_{\text{ref}}(\mu) &= \frac{1}{2} \sum_{k=1}^q w_k \frac{1 + \mu s_k}{(\mu + s_k)^2 + c_k^2}, \quad c_k^2 = 1 - s_k^2 \\ &= \frac{1}{2} \sum_{k=1}^q w_k g_k(\mu), \quad g_k(\mu) \stackrel{\text{def}}{=} \frac{1 + \mu s_k}{(\mu + s_k)^2 + c_k^2}.\end{aligned}$$

Each of the $g_k(\mu)$ s is a rational function with a strictly positive denominator. Simple differentiation shows

$$g'_k(\mu) = -\frac{s_k + 2\mu + s_k\mu^2}{[(\mu + s_k)^2 + c_k^2]^2}.$$

Hence

$$g'_k(1) = -\frac{1}{2(1 + s_k)} < 0 \quad \text{for all } k \implies \rho'_{\text{ref}}(1) = \frac{1}{2} \sum_{k=1}^q w_k g'_k(1) < 0.$$

This establishes (2).

Finally, the formula for $g'_k(\mu)$ shows that if $s_k \geq 0$, then $g'_k(\mu) \leq 0$ for all $\mu \in [0, 1]$. Therefore, for those k s where $1 > s_k \geq 0$, $g_k(\mu)$ are decreasing functions on $[0, 1]$ and $g_k(\mu) \geq g_k(1) = 1/2$ for $\mu \in [0, 1]$. If $s_k < 0$, then

$$g'_k(\mu) = \frac{|s_k|\mu^2 - 2\mu + |s_k|}{[(\mu + s_k)^2 + c_k^2]^2}.$$

The numerator is a convex quadratic that attains its minimum at $\mu = |s_k|^{-1} > 1$. Thus $g'_k(\mu)$ changes sign at most once in $[0, 1]$. But $g'_k(0) = |s_k| > 0$ and $g'_k(1) < 0$ together imply that $g'_k(\mu)$ changes sign exactly once in $[0, 1]$. This means that $g_k(\mu)$ attains a maximum in the interior $(0, 1)$ and attains its minimum in $[0, 1]$ at either $\mu = 0$ or $\mu = 1$. However, $g_k(0) = 1$ while $g_k(1) = 1/2$. Thus we must have $g_k(\mu) \geq 1/2$ for those k s that $s_k < 0$. In conclusion, because $w_k > 0$ and $\min_{\mu \in [0, 1]} g_k(\mu) = g_k(1)$ for all k , $\rho_{\text{ref}}(\mu) \geq \rho_{\text{ref}}(1) = 1/2$. This establishes (3) and completes the proof. \square

Theorem 3.1 shows that the matrix $\rho(M)$, $\rho(\mu) = \rho_{\text{ref}}((\mu - c)/r)$, when applied to a vector, preserves rather well those eigenvectors corresponding to the eigenvalues in \mathcal{I} : those components are never attenuated by a factor smaller than $1/2$. The fact that $\rho'_{\text{ref}}(1) < 0$ shows that $\rho_{\text{ref}}(\mu)$ decreases from $1/2$ at $\mu = 1$ as μ gets larger than 1, as illustrated by Figure 1. As $\rho_{\text{ref}}(\mu)$ is a rational function without poles on the real line, a dense numerical sampling on a finite interval $[0, L]$ gives a good description of $\rho_{\text{ref}}(\mu)$ for $|\mu| \leq L$. The characteristics of action of $\rho(M)$ vectors for eigenvectors corresponding to eigenvalues in $c + \alpha L$, $|\alpha| \leq r$ can be well understood. However, we must ensure that $|\rho_{\text{ref}}(\mu)|$ be small as $|\mu| \rightarrow \infty$ so that $\rho(M)$ does indeed attenuate all eigenvectors that are not of interest. One cannot study the behavior of $\rho_{\text{ref}}(\mu)$ on the entire real line by numerical sampling alone. The next theorem shows that there exists a decreasing function $\xi(\mu)$ on $\mu \in (1, \infty)$ such that $|\rho_{\text{ref}}(\mu)| \leq \xi(\mu)$ for all $\mu > 1$. Furthermore, $\xi(\mu)$ can be evaluated numerically. Thus we can evaluate $\xi(\mu)$ at any point $\mu = L$ to yield a bound on $|\rho_{\text{ref}}(\mu)|$ for all $\mu \geq L$.

THEOREM 3.2. *For a q -point Gauss-Legendre quadrature rule, there exists a function $\xi_q(\mu)$, $\mu \in (1, \infty)$, such that $\xi_q(\mu)$ is decreasing in μ and for any $\mu_0 > 1$, $|\rho_{\text{ref}}(\mu)| \leq \xi_q(\mu_0)$ for all $\mu \geq \mu_0$.*

Proof. Consider a q -point Gauss–Legendre rule. $\rho_{\text{ref}}(\mu)$ is the value obtained by applying this quadrature rule to the definite integral

$$(3.11) \quad \begin{aligned} \pi(\mu) &= \frac{1}{2} \int_{-1}^1 \frac{1 + \mu \sin(\pi t/2)}{1 + 2\mu \sin(\pi t/2) + \mu^2} dt \\ &= \int_{-1}^1 f_\mu(t) dt, \quad f_\mu(t) \stackrel{\text{def}}{=} \frac{1}{2} \frac{1 + \mu \sin(\pi t/2)}{1 + 2\mu \sin(\pi t/2) + \mu^2}. \end{aligned}$$

The subscript μ in f_μ emphasizes that μ is considered a parameter and t is the independent variable. For any fixed $\mu > 1$, $1 + 2\mu \sin(\pi t/2) + \mu^2 > 0$ for all t , and $f_\mu(t)$ is infinitely differentiable (with respect to t). The error in the Gauss–Legendre rule is well known (see, for example, [32]):

$$\int_{-1}^1 f_\mu(t) dt - \rho_{\text{ref}}(\mu) = \frac{f_\mu^{(2q)}(t_0)}{(2q)!} \int_{-1}^1 P_q^2(t) dt$$

for some $t_0 \in (-1, 1)$, and $P_q(t)$ is the monic Legendre polynomial of degree q . It is known [1] that the L^2 -norm of the q -degree Legendre polynomial with the leading coefficient $(\Pi_{j=1}^q (2j-1))/q!$ is $(q+1/2)^{-1/2}$. Therefore,

$$\int_{-1}^1 P_q^2(t) dt = \frac{2^{2q+1}(q!)^4}{(2q+1)((2q)!)^2}.$$

Because $\int_{-1}^1 f_\mu(t) dt = 0$ for $\mu > 1$, we have

$$(3.12) \quad |\rho_{\text{ref}}(\mu)| \leq K_q \max_{t \in [-1, 1]} |f_\mu^{(2q)}(t)|, \quad K_q \stackrel{\text{def}}{=} \frac{2^{2q+1}(q!)^4}{(2q+1)((2q)!)^3}.$$

We will complete the proof by constructing a function

$$\xi_q(\mu) \geq K_q \max_{t \in [-1, 1]} |f_\mu^{(2q)}(t)|,$$

where $\xi_q(\mu)$ is decreasing in μ for $\mu > 1$. This construction is via a simple application of the chain rule. Define

$$F_\mu(s) \stackrel{\text{def}}{=} \frac{1}{2} \frac{1 + \mu s}{1 + 2\mu s + \mu^2} \quad \text{and} \quad s(t) \stackrel{\text{def}}{=} \sin(\pi t/2).$$

Thus $f_\mu(t) = F_\mu(s(t))$. Note that $|s| \leq 1$ for $|t| \leq 1$. Let us first examine the derivative of F_μ (with respect to s). Simple differentiation shows

$$F_\mu^{(k)}(s) = (-1)^{k+1} k! 2^{k-2} \frac{\mu^2 - 1}{(1 + 2s\mu + \mu^2)^{k+1}}.$$

Since (1) $1 + 2s\mu + \mu^2$ is positive and increasing in $\mu \in (1, \infty)$ for any fixed value of $s \in [-1, 1]$, and (2) for any fixed $\mu > 1$, $1 + 2s\mu + \mu^2$ for the range $|s| \leq 1$ attains its minimum value of $1 - 2\mu + \mu^2 = (\mu - 1)^2$ at $s = -1$, we have

$$\max_{s \in [-1, 1]} |F_\mu^{(k)}(s)| = k! 2^{k-2} \frac{\mu^2 - 1}{(\mu - 1)^{2(k+1)}} \stackrel{\text{def}}{=} A_k(\mu).$$

$A_k(\mu)$ as defined above is a decreasing function in $\mu \in (1, \infty)$ as its derivative is easily seen to be always negative. Hence, for any $\mu_0 > 1$

$$(3.13) \quad \max_{s \in [-1, 1]} |F_\mu^{(k)}(s)| \leq A_k(\mu_0) \quad \text{for all } \mu \geq \mu_0.$$

Differentiation of $s(t) = \sin(\pi t/2)$ is simple:

$$|s^{(k)}(t)| = \begin{cases} \left(\frac{\pi}{2}\right)^k |\sin(\pi t/2)| & \text{for } k \text{ even,} \\ \left(\frac{\pi}{2}\right)^k |\cos(\pi t/2)| & \text{for } k \text{ odd.} \end{cases}$$

Note also that, using a half-angle formula,

$$\max_{t \in [-1, 1]} |\sin(\pi t/2) \cos(\pi t/2)| = \max_{t \in [-1, 1]} |\sin(\pi t)/2| = 1/2.$$

We can now construct a bound on the derivative of $f_\mu(t)$. Apply the chain rule formula for higher derivative (often attributed to Faà di Bruno [14]) to the composite function $f_\mu(t) = F_\mu(s(t))$:

$$(3.14) \quad \frac{d^n}{dt^n} F_\mu(s(t)) = \sum_{(k_1, k_2, \dots, k_n) \in \mathcal{S}_n} \frac{n!}{k_1! k_2! \dots k_n!} F_\mu^{(k)}(s) \prod_{j=1}^n \left(\frac{s^{(j)}(t)}{j!} \right)^{k_j},$$

where

$$\mathcal{S}_n = \{ (k_1, k_2, \dots, k_n) \mid k_j \geq 0, k_1 + 2k_2 + 3k_3 + \dots + nk_n = n \}$$

is the set of all nonnegative solutions to the Diophantine equation $k_1 + 2k_2 + \dots + nk_n = n$, and k is defined as $k = \sum_{j=1}^n k_j$. For each solution $(k_1, \dots, k_n) \in \mathcal{S}_n$ we define

$$\begin{aligned} k_{\text{even}} &\stackrel{\text{def}}{=} k_2 + k_4 + \dots + k_{2\lfloor n/2 \rfloor}, \\ k_{\text{odd}} &\stackrel{\text{def}}{=} \left(\sum_{j=1}^n k_j \right) - k_{\text{even}} = k - k_{\text{even}}, \\ k_{\text{sc}} &\stackrel{\text{def}}{=} \min\{k_{\text{even}}, k_{\text{odd}}\}. \end{aligned}$$

Therefore,

$$\begin{aligned} \left| \prod_{j=1}^n \left(\frac{s^{(j)}(t)}{j!} \right)^{k_j} \right| &= \left(\frac{\pi}{2} \right)^{k_1 + 2k_2 + \dots + nk_n} |\sin(\pi t/2)|^{k_{\text{even}}} |\cos(\pi t/2)|^{k_{\text{odd}}} \\ &= \left(\frac{\pi}{2} \right)^n |\sin(\pi t/2)|^{k_{\text{even}}} |\cos(\pi t/2)|^{k_{\text{odd}}} \\ (3.15) \quad &\leq \left(\frac{\pi}{2} \right)^n \left(\frac{1}{2} \right)^{k_{\text{sc}}} \quad \text{for all } t \in [-1, 1]. \end{aligned}$$

Finally, we define

$$\alpha(k_1, k_2, \dots, k_n) \stackrel{\text{def}}{=} \frac{n!}{k_1! k_2! \dots k_n!} \prod_{j=1}^n \left(\frac{1}{j!} \right)^{k_j}$$

and arrive at

$$\begin{aligned} (3.16) \quad \xi_q(\mu) &\stackrel{\text{def}}{=} K_q \left(\frac{\pi}{2} \right)^{2q} \sum_{(k_1, k_2, \dots, k_{2q}) \in \mathcal{S}_{2q}} \alpha(k_1, k_2, \dots, k_{2q}) A_k(\mu) (1/2)^{k_{\text{sc}}}, \\ &\geq K_q \max_{t \in [-1, 1]} |f_\mu^{(2q)}(t)|. \end{aligned}$$

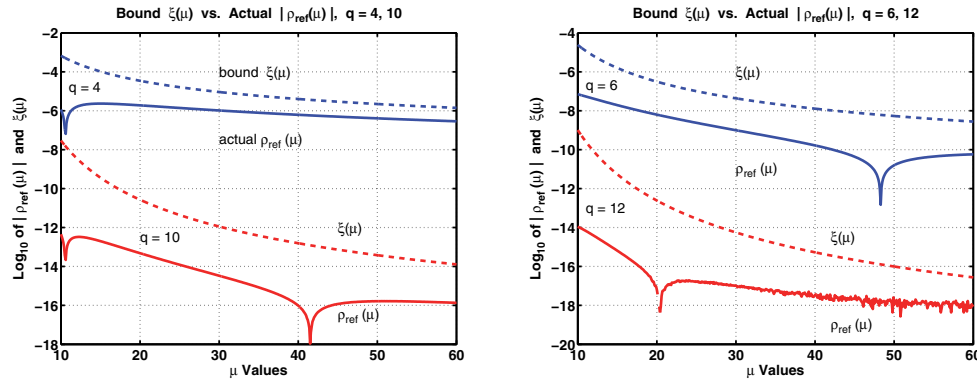


FIG. 3. Upper bound functions that are decreasing are useful in bounding tail ends of $|\rho_{\text{ref}}(\mu)|$. For example, the graph on the left shows $\xi(30) \approx 10^{-12}$ for the $q = 10$ quadrature rule. This implies $|\rho_{\text{ref}}(\mu)| \leq 10^{-12}$ for all $\mu \geq 30$.

This bound is a synthesis of (3.12) through (3.15). The function $\xi_q(\mu)$ is decreasing in μ as each of the $A_k(\mu)$ is a decreasing function. Finally, for any $\mu_0 > 1$, for all $\mu \geq \mu_0$, we have

$$|\rho_{\text{ref}}(\mu)| \leq \xi_q(\mu) \leq \xi_q(\mu_0).$$

This completes the proof. \square

Figure 3 illustrates the upper bound function $\xi_q(\mu)$ for several values of q . Note that $\xi_q(\mu)$ given in (3.16) is easy to compute numerically. Theorem 3.2 allows us to assess the maximum of the infinite tail end $|\rho_{\text{ref}}(\mu)|$ on, for example, $[y, \infty)$ for some specific y by numerical sampling on just a finite interval because

$$\max_{\mu \in [y, \infty)} |\rho_{\text{ref}}(\mu)| \leq \max \left\{ \max_{\mu \in [y, y+L]} |\rho_{\text{ref}}(\mu)|, \xi_q(y+L) \right\}$$

for any $L > 0$. Table 1 tabulates the decay of the tail ends of $\rho_{\text{ref}}(\mu)$ for several specific q -values. It also tabulates the maximum value of $\rho_{\text{ref}}(\mu)$ on the interval $[-1, 1]$.

TABLE 1

For the tabulated quadratures, $1/2 \leq \rho_{\text{ref}}(\mu) \leq 1.024$ for $\mu \in [-1, 1]$ (cf. Theorem 3.1). The rightmost columns show the “relative attenuation” as comparison of $\max_{\mu \in [y, \infty)} |\rho_{\text{ref}}(\mu)|$ with $\min_{\mu \in [-1, 1]} |\rho_{\text{ref}}(\mu)| = 1/2$.

q	$\max_{\mu \in [-1, 1]} \rho_{\text{ref}}(\mu)$	y where $\max_{\mu \in [y, \infty)} \rho_{\text{ref}}(\mu) \leq \frac{1}{2} 10^{-j}, j = 1, 2, \dots, 7$						
		10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-5}	10^{-6}	10^{-7}
4	1.022	1.17	1.84	2.24	6.08	8.96	44.90	145.80
6	1.023	1.08	1.35	1.84	2.32	4.00	5.50	11.39
8	1.024	1.05	1.20	1.45	1.64	2.29	2.59	4.28
10	1.024	1.03	1.13	1.29	1.39	1.74	2.20	2.58
12	1.024	1.03	1.10	1.21	1.28	1.50	1.79	1.96

As stated previously, $M = X\Lambda X^{-1}$ and $\rho(M) = X\rho(\Lambda)X^{-1}$. If $\rho(\lambda) = 1$ for $\lambda \in \text{eig}(M) \cap [\lambda_-, \lambda_+]$ and $\rho(\lambda) = 0$ for $\lambda \in \text{eig}(M) \setminus [\lambda_-, \lambda_+]$, then $\rho(M)$ is the exact subspace projector $X_{\mathcal{T}}X_{\mathcal{T}}^*B$. Table 1 illustrates quantitatively that our construction $\rho(M)$ based on Gaussian–Legendre quadrature is an approximate subspace projector.

For example, for a quadrature rule of $q = 8$ and a general $\mathcal{I} = [\lambda_-, \lambda_+]$ with $c = (\lambda_+ + \lambda_-)/2$, $r = (\lambda_+ - \lambda_-)/2$, we have $1 \approx \rho(\lambda) \in [1/2, 1.024]$ for $\lambda \in \mathcal{I}$ and $|\rho(\lambda)| \leq \frac{1}{2} 10^{-3}$ for $|\lambda - c| \geq 1.45r$.

4. Robust subspace convergence of FEAST. The previous analysis suggests that a Gauss–Legendre quadrature accelerator $\rho(M)$ should be effective in Algorithm A as the eigenvalues of interest of M are now the (highly) dominant eigenvalues of $\rho(M)$. We restate Algorithm A as Algorithm FEAST, with $\rho(M)$ being derived specifically from Gauss–Legendre quadratures using a circular path parametrized as in (3.2). A variety of functions ρ can be constructed by different quadrature rules (e.g., the trapezoidal rule) on different contours (e.g., ellipses). It is also possible to construct ρ from a pure function approximation approach, for example, via Zolotarev approximation [33].

Algorithm FEAST. As given in [21]

- 1: Specify $\mathcal{I} = [\lambda_-, \lambda_+]$ and a Gauss–Legendre quadrature choice of q .
 - 2: Pick p and p random n -vectors $Q_{(0)} = [q_1, q_2, \dots, q_p]$. Set $k \leftarrow 1$.
 - 3: **repeat**
 - 4: Approximate subspace projection (see (3.7)): $Y_{(k)} \leftarrow \rho(M) \cdot Q_{(k-1)}$.
 - 5: Form reduced system: $\hat{A}_{(k)} \leftarrow Y_{(k)}^* A Y_{(k)}$, $\hat{B}_{(k)} \leftarrow Y_{(k)}^* B Y_{(k)}$.
 - 6: Solve p -dimension eigenproblem: $\hat{A}_{(k)} \hat{X}_{(k)} = \hat{B}_{(k)} \hat{X}_{(k)} \hat{\Lambda}_{(k)}$ for $\hat{\Lambda}_{(k)}$, $\hat{X}_{(k)}$.
 - 7: Set $Q_{(k)} \leftarrow Y_{(k)} \hat{X}_{(k)}$, in particular $Q_{(k)}^* B Q_{(k)} = I_p$.
 - 8: $k \leftarrow k + 1$.
 - 9: **until** Appropriate stopping criteria
-

Basic convergence properties of subspace iteration for eigenvalue problems are well known (see, for example, [6, 25]). Nonetheless, utilization of an approximate subspace projector leads to special properties. $\rho(M)$ approximates a low-rank operator, and thus we customize our analysis to focus on subspaces within the generated subspace $\mathcal{Q}_{(k)} = \text{span}(Q_{(k)})$. The first theorem in this section, Theorem 4.1, generalizes Theorem 5.2 of [25] to cover generalized eigenvalue problems. Our second theorem, Theorem 4.4, takes into account that the application of $\rho(M)$ is inexact as it involves solutions of linear systems. We show that subspace convergence is not affected in any fundamental way, which accounts for this section's robust convergence title.

As the decay of the function $\rho(\mu)$ is closely tied to the property of the approximate subspace projector $\rho(M)$, we adopt the following convention. Whenever there is an underlying fixed choice of $\rho(M)$, we number the eigenpairs $(\lambda_j, \mathbf{x}_j)$ so that $|\rho(\lambda_1)| \geq |\rho(\lambda_2)| \geq \dots \geq |\rho(\lambda_n)|$. In particular, if there are e eigenvalues in \mathcal{I} , then

$$\rho(\lambda_1) \geq \rho(\lambda_2) \geq \dots \geq \rho(\lambda_e) \geq 1/2 > |\rho(\lambda_{e+1})| \geq \dots \geq |\rho(\lambda_n)|.$$

We denote the eigenvalues of $\rho(M)$ by $\gamma_j \stackrel{\text{def}}{=} \rho(\lambda_j)$, $j = 1, 2, \dots, n$. Our analysis involves examining sections of the eigenvectors $X = [\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n]$ and their corresponding eigenvalues. We set up some simplifying notation: For any integer ℓ , $1 \leq \ell < n$,

$$\begin{aligned} X_\ell &= [\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_\ell], & X_{\ell'} &= [\mathbf{x}_{\ell+1}, \mathbf{x}_{\ell+2}, \dots, \mathbf{x}_n], \\ \Lambda_\ell &= \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_\ell), & \Lambda_{\ell'} &= \text{diag}(\lambda_{\ell+1}, \lambda_{\ell+2}, \dots, \lambda_n), \\ \Gamma_\ell &= \text{diag}(\gamma_1, \gamma_2, \dots, \gamma_\ell), & \Gamma_{\ell'} &= \text{diag}(\gamma_{\ell+1}, \gamma_{\ell+2}, \dots, \gamma_n). \end{aligned}$$

With this notation, $X_\ell X_\ell^* B$ is the B -orthogonal projector onto $\text{span}(\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_\ell\})$, $X_{\ell'} X_{\ell'}^* B$ is the B -orthogonal projector onto $\text{span}(\{\mathbf{x}_{\ell+1}, \mathbf{x}_{\ell+2}, \dots, \mathbf{x}_n\})$, $I = X_\ell X_\ell^* B + X_{\ell'} X_{\ell'}^* B$, and

$$(4.1) \quad \rho(M) = X_\ell \Gamma_\ell X_\ell^* B + X_{\ell'} \Gamma_{\ell'} X_{\ell'}^* B.$$

All norms $\|\cdot\|$, unless explicitly stated using subscripts, are 2-norms.

THEOREM 4.1. *Consider Algorithm FEAST. Suppose $|\gamma_p| > 0$ and that the $p \times p$ matrix $X_p^* B Q_{(0)}$ is invertible. Let m be any integer $m \leq p$. Then there is a constant α such that the following hold for $k = 1, 2, \dots$:*

- The subspace $\mathcal{Q}_{(k)} \stackrel{\text{def}}{=} \text{span}(Q_{(k)})$ is of dimension p .
- $Q_{(k)}$ is of the form $Q_{(k)} = [(X_m + X_{p'} E_{(k)}) L_{(k)}^{-1}, V_{(k)}] U_{(k)}$, where $U_{(k)}$ is a $p \times p$ unitary matrix. $E_{(k)}, L_{(k)}, V_{(k)}$ are of conforming dimensions of $(n-p) \times m, m \times m, n \times (p-m)$, respectively. ($V_{(k)}$ is nonexistent for $m = p$.) Moreover, $E_{(k)} = \Gamma_{p'} E_{(k-1)} \Gamma_m^{-1}$.
- For each $j = 1, 2, \dots, m$, there is a vector $\mathbf{s}_j \in \mathcal{Q}_{(k)}$ such that $\|\mathbf{x}_j - \mathbf{s}_j\|_B \leq \alpha |\gamma_{p+1}/\gamma_j|^k$. The B -norm of an n -vector \mathbf{y} is defined in the standard way: $\|\mathbf{y}\|_B \stackrel{\text{def}}{=} (\mathbf{y}^* B \mathbf{y})^{1/2}$. In particular, $\|(I - P_{(k)}) \mathbf{x}_j\|_B \leq \alpha |\gamma_{p+1}/\gamma_j|^k$, where $P_{(k)}$ is the B -orthogonal projection onto the space $\mathcal{Q}_{(k)}$.

Proof. $|\gamma_p| > 0$ implies that Γ_i is invertible for any $i = 1, 2, \dots, p$. Suppose $X_p^* B Q_{(k-1)}$ is invertible for some $k = 1, 2, \dots$. Then

$$\begin{aligned} Y_{(k)} &= \rho(M) Q_{(k-1)} \\ &= X_p \Gamma_p (X_p^* B Q_{(k-1)}) + X_{p'} \Gamma_{p'} (X_{p'}^* B Q_{(k-1)}) \\ &= (X_p + X_{p'} (\Gamma_{p'} X_{p'}^* B Q_{(k-1)}) Z^{-1}) Z, \end{aligned}$$

where $Z = \Gamma_p (X_p^* B Q_{(k-1)})$ is invertible. Thus $Y_{(k)}$ has full column rank, which implies $\hat{B}_{(k)} = Y_{(k)}^* B Y_{(k)}$ is Hermitian positive definite. The dimension- p generalized eigenvalue problem specified by $\hat{A}_{(k)}$ and $\hat{B}_{(k)}$ has linearly independent eigenvectors; that is, the matrix $\hat{X}_{(k)}$ is invertible. Consequently, $Q_{(k)} = Y_{(k)} \hat{X}_{(k)}$ has full column rank, $\mathcal{Q}_{(k)}$ is of dimension p , and the matrix $X_p^* B Q_{(k)}$ is invertible. Since by assumption $X_p^* B Q_{(0)}$ is invertible, we conclude by induction that the subspaces $\mathcal{Q}_{(k)}$ are all of dimension p for $k = 1, 2, \dots$.

Define $U_{(0)} \stackrel{\text{def}}{=} X_p^* B Q_{(0)}$. $U_{(0)}$ is invertible by assumption (but not necessarily unitary):

$$\begin{aligned} Q_{(0)} &= (X_p X_p^* B + X_{p'} X_{p'}^* B) Q_{(0)} \\ &= (X_p + X_{p'} X_{p'}^* B Q_{(0)} U_{(0)}^{-1}) U_{(0)}. \end{aligned}$$

Given an integer $m \leq p$, partition the p columns of $Q_{(0)} U_{(0)}^{-1}$ into m and $p-m$ columns:

$$Q_{(0)} = [(X_m + X_{p'} E_{(0)}), V_{(0)}] U_{(0)},$$

where $E_{(0)}$ is simply the first m columns of $X_{p'}^* B Q_{(0)} U_{(0)}^{-1}$. Consequently,

$$Y_{(1)} = \rho(M) Q_{(0)} = [(X_m + X_{p'} E_{(1)}) \Gamma_m, \rho(M) V_{(0)}] U_{(0)},$$

$E_{(1)} = \Gamma_{p'} E_{(0)} \Gamma_m^{-1}$. $X_m + X_{p'} E_{(1)}$ is of full rank m as X_m is linearly independent with $X_{p'}$. Since B is Hermitian positive definite, there is a matrix $L_{(1)}$ such that

$$L_{(1)}^* L_{(1)} = (X_m + X_{p'} E_{(1)})^* B (X_m + X_{p'} E_{(1)}),$$

which implies $(X_m + X_{p'}E_{(1)})L_{(1)}^{-1}$ is B -orthonormal. Any $L_{(1)}$ that satisfies the above equation is acceptable. Note that $L_{(1)}$ is unique up to a unitary equivalence. For any specifically chosen $L_{(1)}$, complete a B -orthonormal basis for $\text{span}(Y_{(1)})$ to yield $[(X_m + X_{p'}E_{(1)})L_{(1)}^{-1} \quad V_{(1)}]$. Since $Q_{(1)}$ is B -orthonormal as well, there must be a $p \times p$ unitary matrix $U_{(1)}$ such that

$$Q_{(1)} = [(X_m + X_{p'}E_{(1)})L_{(1)}^{-1}, \quad V_{(1)}] U_{(1)}.$$

We have shown that at $k = 1$, $Q_{(k)}$ is of the form

$$(4.2) \quad Q_{(k)} = [(X_m + X_{p'}E_{(k)})L_{(k)}^{-1}, \quad V_{(k)}] U_{(k)},$$

where $U_{(k)}$ is unitary and $Q_{(k)}$ B -orthonormal. Suppose now that (4.2) holds for some $k \geq 1$:

$$Y_{(k+1)} = \rho(M)Q_{(k)} = [(X_m + X_{p'}E_{(k+1)})\Gamma_m L_{(k)}^{-1} \quad \rho(M)V_{(k)}] U_{(k)},$$

where

$$E_{(k+1)} = \Gamma_{p'} E_{(k)} \Gamma_m^{-1}.$$

Let $L_{(k+1)}$ be such that

$$L_{(k+1)}^* L_{(k+1)} = (X_m + X_{p'}E_{(k+1)})^* B (X_m + X_{p'}E_{(k+1)}).$$

This makes $(X_m + X_{p'}E_{(k+1)})L_{(k+1)}^{-1}$ B -orthonormal. Complete a B -orthonormal basis with $V_{(k+1)}$ for $\text{span}(Y_{(k+1)}) = \text{span}(Q_{(k+1)})$. Hence, there must be a $p \times p$ unitary matrix $U_{(k+1)}$ such that

$$Q_{(k+1)} = [(X_m + X_{p'}E_{(k+1)})L_{(k+1)}^{-1}, \quad V_{(k+1)}] U_{(k+1)}.$$

By induction, we have established the second item of this theorem.

Finally, each of the m column vectors of $X_m + X_{p'}E_{(k)}$ is in the subspace $\mathcal{Q}_{(k)}$, and $E_{(k)} = \Gamma_{p'}^k E_{(0)} \Gamma_m^{-k}$ for $k = 1, 2, \dots$. Let $\alpha \stackrel{\text{def}}{=} \|E_{(0)}\|$. For each $k = 1, 2, \dots$, and $j = 1, 2, \dots, m$, let e_j be the j th column of $E_{(k)}$, and define $s_j \stackrel{\text{def}}{=} x_j + X_{p'}e_j$. Clearly $s_j \in \mathcal{Q}_{(k)}$ and

$$\|x_j - s_j\|_B = \|X_{p'}e_j\|_B = \|e_j\| \leq \alpha \left| \frac{\gamma_{p+1}}{\gamma_j} \right|^k.$$

In particular,

$$\|(I - P_{(k)})x_j\|_B = \min_{s \in \mathcal{Q}_{(k)}} \|x_j - s\|_B \leq \alpha \left| \frac{\gamma_{p+1}}{\gamma_j} \right|^k.$$

This proves the final item of the theorem. \square

Theorem 4.1 together with Table 1 illustrates the effectiveness of FEAST. For example, let $\mathcal{I} = [\lambda_-, \lambda_+]$ be the specified interval, with center $c = (\lambda_+ + \lambda_-)/2$ and radius $r = (\lambda_+ - \lambda_-)/2$. If M 's spectrum is distributed somewhat uniformly, then the interval $[c - 1.45r, c + 1.45r]$ would have roughly 1.45 times as many eigenvalues as there are in \mathcal{I} . For a quadrature rule of $q = 8$ and a p that happens to be $p \geq 1.45e$,

we would expect for $j = 1, 2, \dots, e$, that $|\gamma_{p+1}/\gamma_j|$ be as small as 10^{-3} . So that for each j , there exist elements $\mathbf{s}_{(k)} \in \mathcal{Q}_{(k)}$, $k = 1, 2, \dots$, such that $\|\mathbf{x}_j - \mathbf{s}_{(k)}\|_B \rightarrow 0$ at a rate of 10^{-3k} .

Application of $\rho(M)$ in general incurs more errors compared to standard subspace iterations ($\rho(\mu) \equiv 1$) or a low-degree polynomial accelerator ($\rho(\mu)$ is a low-degree polynomial). We now examine Algorithm FEAST when step 4 is replaced by

$$Y_{(k)} \leftarrow \rho(M)Q_{(k-1)} + \Delta_{(k-1)}, \quad \Delta_{(k-1)} \text{ is a } n \times p \text{ matrix.}$$

Our analysis below shows that convergence is not affected in any fundamental way. Without the error term, Theorem 4.1 shows that the generated subspaces $\mathcal{Q}_{(k)}$ contains elements of the form $\mathbf{x}_j + X_{p'}\mathbf{e}$, $1 \leq j \leq m$. The component $X_{p'}\mathbf{e}$ will be attenuated in the iterative process. The presence of the error term $\Delta_{(k)}$ in effect introduces a small component of the form $X_{m'}\mathbf{f}$ at each iteration. Once introduced, however, this component will also be attenuated as the iterative process proceeds. Roughly speaking, the dominant error term is the one most recently introduced, and convergence of subspace iteration remains robust. The next lemma examines the form of the generated subspaces and Theorem 4.4 quantifies them.

LEMMA 4.2. *Suppose for any $k = 1, 2, \dots$, $Q_{(k-1)}$ is of the form*

$$[(X_m + X_{p'}E_{(k-1)} + X_{m'}F_{(k-1)})L_{(k-1)}^{-1}, V_{(k-1)}]U_{(k-1)}$$

for some $m \leq p$, where $U_{(k-1)}$ and $L_{(k-1)}$ are invertible matrices of dimensions $p \times p$ and $m \times m$, respectively. The matrices $E_{(k-1)}$, $F_{(k-1)}$, and $V_{(k-1)}$ are of conforming dimensions. Define the terms $\xi_{(k-1)}$, $\zeta_{(k-1)}$, $\psi_{(k-1)}$ via the following partitioning involving the error term $\Delta_{(k-1)}$:

$$X^{-1}\Delta_{(k-1)}U_{(k-1)}^{-1} \left[\begin{array}{c|c} L_{(k-1)} & I \end{array} \right] = \left[\begin{array}{c|c} \xi_{(k-1)} & \psi_{(k-1)} \end{array} \right], \quad \xi_{(k-1)} \text{ is } m \times m.$$

If $\Gamma_m + \xi_{(k-1)}$ is invertible and $Y_{(k)} = \rho(M)Q_{(k-1)} + \Delta_{(k-1)}$ remains full column rank, then $Q_{(k)}$ is of the form

$$Q_{(k)} = [(X_m + X_{p'}E_{(k)} + X_{m'}F_{(k)})L_{(k)}^{-1}, V_{(k)}]U_{(k)},$$

where $U_{(k)}$ is unitary, and

$$L_{(k)}^* L_{(k)} = (X_m + X_{p'}E_{(k)} + X_{m'}F_{(k)})^* B (X_m + X_{p'}E_{(k)} + X_{m'}F_{(k)}).$$

In particular, $\|L_{(k)}\| \leq (1 + (\|E_{(k)}\| + \|F_{(k)}\|)^2)^{1/2}$. Furthermore,

$$\begin{aligned} E_{(k)} &= \Gamma_{p'} E_{(k-1)} (\Gamma_m + \xi_{(k-1)})^{-1} \quad \text{and} \\ F_{(k)} &= \Gamma_{m'} F_{(k-1)} (\Gamma_m + \xi_{(k-1)})^{-1} + \zeta_{(k-1)} (\Gamma_m + \xi_{(k-1)})^{-1}. \end{aligned}$$

Proof. By assumption,

$$\begin{aligned} &\rho(M)Q_{(k-1)} \\ &= [(X_m \Gamma_m + X_{p'} \Gamma_{p'} E_{(k-1)} + X_{m'} \Gamma_{m'} F_{(k-1)})L_{(k-1)}^{-1} \quad \rho(M)V_{(k-1)}]U_{(k-1)}, \\ &\Delta_{(k-1)} \\ &= [(X_m \xi_{(k-1)} + X_{m'} \zeta_{(k-1)})L_{(k-1)}^{-1} \quad X\psi_{(k-1)}]U_{(k-1)}. \end{aligned}$$

The following m column vectors are in $\text{span}(Y_{(k)})$, $Y_{(k)} = \rho(M) Q_{(k-1)} + \Delta_{(k-1)}$:

$$\begin{aligned} X_m (\Gamma_m + \xi_{(k-1)}) + X_{p'} \Gamma_{p'} E_{(k-1)} + X_{m'} (\Gamma_{m'} F_{(k-1)} + \zeta_{(k-1)}) \\ = (X_m + X_{p'} E_{(k)} + X_{m'} F_{(k)}) (\Gamma_m + \xi_{(k-1)}), \end{aligned}$$

where

$$\begin{aligned} E_{(k)} &= \Gamma_{p'} E_{(k-1)} (\Gamma_m + \xi_{(k-1)})^{-1} \quad \text{and} \\ F_{(k)} &= \Gamma_{m'} F_{(k-1)} (\Gamma_m + \xi_{(k-1)})^{-1} + \zeta_{(k-1)} (\Gamma_m + \xi_{(k-1)})^{-1}. \end{aligned}$$

We can B -orthonormalize these m columns via

$$(X_m + X_{p'} E_{(k)} + X_{m'} F_{(k)}) L_{(k)}^{-1},$$

where

$$L_{(k)}^* L_{(k)} = (X_m + X_{p'} E_{(k)} + X_{m'} F_{(k)})^* B (X_m + X_{p'} E_{(k)} + X_{m'} F_{(k)}).$$

Recall that $B = C^* C$ and CX is unitary. Therefore,

$$\begin{aligned} \|L_{(k)}\|^2 &\leq \|(X_m + X_{p'} E_{(k)} + X_{m'} F_{(k)})^* B (X_m + X_{p'} E_{(k)} + X_{m'} F_{(k)})\| \\ &\leq 1 + 2\|E_{(k)}\| \|F_{(k)}\| + \|E_{(k)}\|^2 + \|F_{(k)}\|^2 \\ &= 1 + (\|E_{(k)}\| + \|F_{(k)}\|)^2. \end{aligned}$$

Complete a B -orthonormal basis for $\text{span}(Y_{(k)})$ by adding an appropriate $p-m$ column $V_{(k)}$. Since $Q_{(k)}$ is B -orthonormal for $k = 1, 2, \dots$, there is a $p \times p$ unitary matrix $U_{(k)}$ such that

$$Q_{(k)} = [(X_m + X_{p'} E_{(k)} + X_{m'} F_{(k)}) L_{(k)}^{-1}, V_{(k)}] U_{(k)}.$$

This completes the proof. \square

The next lemma is a collection of several technical details needed in subsequent discussions.

LEMMA 4.3. Assume $|\gamma_p| > 0$ and consider any integer $m \leq p$. Let $\alpha, \beta, \beta', \delta$ be positive numbers where

$$\delta < 1, \quad \beta(1 + \delta) \leq 1/2, \quad \tau \stackrel{\text{def}}{=} 1 - \beta'(1 + \delta) > 0.$$

Define the sequence $e_{\delta,0} \stackrel{\text{def}}{=} \alpha$, $f_{\delta,0} \stackrel{\text{def}}{=} 0$, and for $k = 1, 2, \dots$,

$$e_{\delta,k} \stackrel{\text{def}}{=} \beta(1 + \delta)e_{\delta,k-1}, \quad f_{\delta,k} \stackrel{\text{def}}{=} \beta'(1 + \delta)f_{\delta,k-1} + \delta(1 + \delta)/2.$$

The following hold:

- (1) $e_{\delta,k} = \alpha(\beta(1 + \delta))^k$ decreases as k increases. As long as $e_{\delta,k-1} \geq 2\delta$, $e_{\delta,k} + f_{\delta,k} \leq e_{\delta,k-1} + f_{\delta,k-1}$.
- (2) $f_{\delta,k} \leq \delta(1 + \delta)/(2\tau)$ for all $k = 1, 2, \dots$.
- (3) Consider any $m \times m$ matrix ξ . If $\|\xi\| \leq \delta|\gamma_m|/2$, then $\|(I + \Gamma_m^{-1}\xi)^{-1}\| < 1 + \delta$, $\|(I + \Gamma_m^{-1}\xi)^{-1} - I\| < \delta$, and the matrix $\Gamma_m + \xi$ is invertible with $(\Gamma_m + \xi)^{-1} = (I + \Gamma_m^{-1}\xi)^{-1} \Gamma_m^{-1}$.

- (4) Consider a Hermitian matrix of an arbitrary dimension ℓ of the forms $I + \xi$, $\xi^* = \xi$, and $\|\xi\| \leq 1/2$. Then $(I + \xi)^{1/2}$ and $(I + \xi)^{-1/2}$ are well defined and

$$\|(I + \xi)^{\pm 1/2} - I\| \leq \|\xi\|.$$

Proof. We prove $e_{\delta,k} = \alpha(\beta(1 + \delta))^k$ is clear, and $e_{\delta,k}$ is obviously a decreasing function in k because $\beta(1 + \delta) \leq 1/2$ by assumption. For $k \geq 1$ and $e_{\delta,k-1} \geq 2\delta$, we have

$$\begin{aligned} e_{\delta,k} + f_{\delta,k} &= \beta(1 + \delta)e_{\delta,k-1} + \beta'(1 + \delta)f_{\delta,k-1} + \delta(1 + \delta)/2 \\ &\leq e_{\delta,k-1}/2 + f_{\delta,k-1} + \delta(1 + \delta)/2 \quad \text{as } \beta(1 + \delta) \leq 1/2 \text{ and } \beta'(1 + \delta) < 1 \\ &\leq e_{\delta,k-1}/2 + f_{\delta,k-1} + \delta \quad \text{as } \delta < 1 \\ &\leq e_{\delta,k-1}/2 + f_{\delta,k-1} + e_{\delta,k-1}/2 \quad \text{as } e_{\delta,k-1} \geq 2\delta \\ &= e_{\delta,k-1} + f_{\delta,k-1}. \end{aligned}$$

This proves (1).

Next,

$$f_{\delta,k} < \frac{\delta}{2}(1 + \delta) \sum_{\ell=0}^{\infty} (\beta'(1 + \delta))^{\ell} \leq \frac{\delta(1 + \delta)}{2(1 - \beta'(1 + \delta))} = \frac{\delta(1 + \delta)}{2\tau},$$

which proves (2).

To prove (3), note that $\|\xi\| \leq \delta|\gamma_m|/2$ implies $\|\Gamma_m^{-1}\xi\| \leq \frac{\delta}{2} < 1/2$. Consequently, $(I + \Gamma_m^{-1}\xi)^{-1} = \sum_{\ell=0}^{\infty} (-1)^{\ell} (\Gamma_m^{-1}\xi)^{\ell}$ and

$$\|(I + \Gamma_m^{-1}\xi)^{-1}\| = \left\| \sum_{\ell=0}^{\infty} (-1)^{\ell} (\Gamma_m^{-1}\xi)^{\ell} \right\| \leq 1 + \frac{\delta}{2} \sum_{\ell=0}^{\infty} \left(\frac{\delta}{2}\right)^{\ell} < 1 + \delta.$$

Similarly,

$$\|(I + \Gamma_m^{-1}\xi)^{-1} - I\| = \left\| \sum_{\ell=1}^{\infty} (-1)^{\ell} (\Gamma_m^{-1}\xi)^{\ell} \right\| \leq \frac{\delta}{2} \sum_{\ell=0}^{\infty} \left(\frac{\delta}{2}\right)^{\ell} < \delta.$$

Moreover, $\Gamma_m + \xi = \Gamma_m (I + \Gamma_m^{-1}\xi)$ must be invertible as $(\Gamma_m + \xi)^{-1} = (I + \Gamma_m^{-1}\xi)^{-1} \Gamma_m^{-1}$.

Finally, $\|\xi\| \leq 1/2$ implies $\|I + \xi\| \in [1 - \|\xi\|, 1 + \|\xi\|] \subseteq [1/2, 3/2]$. Thus $I + \xi$ is Hermitian positive definite, with an eigendecomposition ZDZ^* , $D = \text{diag}(d_1, d_2, \dots, d_{\ell})$, $d_j \in [1/2, 3/2]$ for all $j = 1, 2, \dots, \ell$. $(I + \xi)^{\pm 1/2} = Z D^{\pm 1/2} Z^*$. Therefore,

$$\|(I + \xi)^{1/2} - I\| = \|D^{1/2} - I\| \leq \max_{|x| \leq \|\xi\|} |(1 + x)^{1/2} - 1| \leq \|\xi\|,$$

where the last inequality holds because of $\|\xi\| \leq 1/2$. Similarly,

$$\|(I + \xi)^{-1/2} - I\| = \|D^{-1/2} - I\| \leq \max_{|x| \leq \|\xi\|} |(1 + x)^{-1/2} - 1| \leq \|\xi\|,$$

where the last inequality holds because of $\|\xi\| \leq 1/2$. This completes the proof of the lemma. \square

THEOREM 4.4. *Consider Algorithm FEAST, where application of $\rho(M)$ to Q results in $\rho(M)Q + \Delta$. Specifically, step 4 of FEAST becomes $Y_{(k)} \leftarrow \rho(M)Q_{(k-1)} + \Delta_{(k-1)}$. Suppose $|\gamma_p| > 0$, $U_{(0)} \stackrel{\text{def}}{=} X_p^* B Q_{(0)}$ is invertible, and that $Q_{(k)}$ for all k have dimension p even in the presence of errors $\Delta_{(k)}$ s. Let m be any integer $m \leq p$ and let $E_{(0)}$ be the $(n-p) \times m$ matrix, the first m columns of $(X_p^* B Q_{(0)}) U_{(0)}^{-1}$. Define $\alpha \stackrel{\text{def}}{=} \|E_{(0)}\|$. Suppose there is a constant δ , $0 < \delta < 1$ such that the computational errors $\Delta_{(k)}$ always satisfy*

$$\|\Delta_{(k)}\| < \min \left\{ \frac{\delta |\gamma_m|}{2 \|C\| \|U_{(0)}^{-1}\|}, \frac{\delta |\gamma_m|}{2 \|C\| \sqrt{1 + \alpha^2}} \right\},$$

and such that $|\gamma_{p+1}/\gamma_m|(1+\delta) \leq 1/2$ and $\tau \stackrel{\text{def}}{=} 1 - |\gamma_{m+1}/\gamma_m|(1+\delta) > 0$. Define the sequence $e_{\delta,k}, f_{\delta,k}$, $k = 0, 1, 2, \dots$, as in Lemma 4.3 using the α and δ here, and $|\gamma_{p+1}/\gamma_m|$ as β , $|\gamma_{m+1}/\gamma_m|$ as β' . The following hold.

- (1) For $k = 1$, as well as for all subsequent $k = 2, 3, \dots$, as long as $e_{\delta,k-1} \geq 2\delta$,

$$Q_{(k)} = [(X_m + X_{p'} E_{(k)} + X_{m'} F_{(k)}) L_{(k)}^{-1}, V_{(k)}] U_{(k)},$$

where $U_{(k)}$ is unitary of dimension $p \times p$,

$$E_{(k)} = \Gamma_{p'} E_{(k-1)} (\Gamma_m + \xi_{(k-1)})^{-1} \quad \text{and}$$

$$F_{(k)} = \Gamma_{m'} F_{(k-1)} (\Gamma_m + \xi_{(k-1)})^{-1} + \zeta_{(k-1)} (\Gamma_m + \xi_{(k-1)})^{-1}.$$

Furthermore, $\|E_{(k)}\| \leq e_{\delta,k}$ and $\|F_{(k)}\| \leq f_{\delta,k}$.

- (2) For $k = 1$, as well as for all subsequent $k = 2, 3, \dots$, as long as $e_{\delta,k-1} \geq 2\delta$, there are m vectors $\mathbf{s}_j \in Q_{(k)}$, $j = 1, 2, \dots, m$, such that

$$\|\mathbf{x}_j - \mathbf{s}_j\|_B \leq \alpha \left(\left| \frac{\gamma_{p+1}}{\gamma_m} \right| (1 + \delta) \right)^k + \frac{\delta(1 + \delta)}{2\tau},$$

and also, alternatively,

$$\|\mathbf{x}_j - \mathbf{s}_j\|_B \leq \alpha \left| \frac{\gamma_{p+1}}{\gamma_j} \right|^k + \alpha \delta \left| \frac{\gamma_{p+1}}{\gamma_m} \right|^k \sum_{\ell=0}^{k-1} (1 + \delta)^\ell + \frac{\delta(1 + \delta)}{2\tau}.$$

Both bounds hold with $\|\mathbf{x}_j - \mathbf{s}_j\|_B$ replaced by $\|(I - P_{(k)})\mathbf{x}_j\|_B$.

Proof. From definitions of $E_{(0)}$ and $U_{(0)}$,

$$Q_{(0)} = [X_m + X_{p'} E_{(0)} + X_{m'} F_{(0)}, V_{(0)}] U_{(0)},$$

$$\Delta_{(0)} = [X_m \xi_{(0)} + X_{m'} \zeta_{(0)}, X \psi_{(0)}] U_{(0)},$$

where $F_{(0)}$ is the zero matrix of dimension $(n-m) \times m$,

$$X^{-1} \Delta_{(0)} U_{(0)}^{-1} = \left[\begin{array}{c} \xi_{(0)} \\ \zeta_{(0)} \end{array} \middle| \psi_{(0)} \right].$$

Because $\|\xi_{(0)}\|, \|\zeta_{(0)}\| \leq \|C\| \|\Delta_{(0)}\| \|U_{(0)}^{-1}\| < \delta |\gamma_m|/2$, Lemma 4.3 shows that $\Gamma_m + \xi_{(0)}$ is invertible. Lemma 4.2 shows that (1) holds for $k = 1$. We use an induction argument. Suppose the following hold for $k = 1, 2, \dots, K-1$ for some $K \geq 2$:

$$(4.3) \quad \begin{aligned} Q_{(k)} &= [(X_m + X_{p'} E_{(k)} + X_{m'} F_{(k)}) L_{(k)}^{-1}, V_{(k)}] U_{(k)}, \\ E_{(k)} &= \Gamma_{p'} E_{(k-1)} (\Gamma_m + \xi_{(k-1)})^{-1}, \\ F_{(k)} &= \Gamma_{m'} F_{(k-1)} (\Gamma_m + \xi_{(k-1)})^{-1} + \zeta_{(k-1)} (\Gamma_m + \xi_{(k-1)})^{-1}, \end{aligned}$$

where $\|L_{(k)}\| \leq \sqrt{1 + (e_{\delta,k} + f_{\delta,k})^2}$, $\|E_{(k)}\| \leq e_{\delta,k}$, $\|F_{(k)}\| \leq f_{\delta,k}$. Suppose $e_{\delta,K-1} \geq 2\delta$; then $e_{\delta,K-2} \geq 2\delta$. Lemma 4.3 shows that $e_{\delta,K-1} + f_{\delta,K-1} \leq e_{\delta,K-2} + f_{\delta,K-2} \leq \dots \leq e_{\delta,0} + f_{\delta,0} = \alpha$. Consequently, $\|L_{(K-1)}\| \leq \sqrt{1 + \alpha^2}$. Examining the partition

$$X^{-1} \Delta_{(K-1)} U_{(K-1)}^{-1} \left[\frac{L_{(K-1)}}{I} \right] = \left[\begin{array}{c|c} \xi_{(K-1)} & \psi_{(K-1)} \\ \hline \zeta_{(K-1)} & \end{array} \right],$$

and noting that $U_{(k)}$ are all unitary for $k \geq 1$, we conclude that

$$\begin{aligned} \|\xi_{(K-1)}\|, \|\zeta_{(K-1)}\| &\leq \|C\| \|\Delta_{(K-1)}\| \|L_{(K-1)}\| \\ &\leq \|C\| \|\Delta_{(K-1)}\| \sqrt{1 + \alpha^2} \\ &< \delta |\gamma_m|/2. \end{aligned}$$

Lemma 4.3 shows that $\Gamma_m + \xi_{(K-1)}$ is invertible. And hence by Lemma 4.2, (4.3) holds for $k = K$ as well. Furthermore,

$$\begin{aligned} \|E_{(K)}\| &\leq |\gamma_{p+1}| \|E_{(K-1)}\| \|(I + \Gamma_m^{-1} \xi_{(K-1)})^{-1}\| \|\Gamma_m^{-1}\| \\ &\leq |\gamma_{p+1}/\gamma_m| (1 + \delta) e_{\delta,K-1} \\ &= e_{\delta,K}, \\ \|F_{(K)}\| &\leq |\gamma_{m+1}/\gamma_m| (1 + \delta) \|F_{(K-1)}\| + \delta(1 + \delta)/2 \\ &\leq |\gamma_{m+1}/\gamma_m| (1 + \delta) f_{\delta,K-1} + \delta(1 + \delta)/2 \\ &= f_{\delta,K}. \end{aligned}$$

This establishes the first point of the theorem.

For $k = 1, 2, \dots$, and as long as $e_{\delta,k-2} \geq 2\delta$, let \mathbf{s}_j be the j th column of $X_m + X_{p'}E_{(k)} + X_{m'}F_{(k)}$. The first bound is easy to obtain:

$$\begin{aligned} \|\mathbf{x}_j - \mathbf{s}_j\|_B &\leq \|X_{p'}E_{(k)} + X_{m'}F_{(k)}\|_B \\ &\leq \|X_{p'}E_{(k)}\|_B + \|X_{m'}F_{(k)}\|_B \\ &= \|E_{(k)}\| + \|F_{(k)}\| \\ &\leq e_{\delta,k} + f_{\delta,k} \\ &\leq \alpha \left(\left| \frac{\gamma_{p+1}}{\gamma_m} \right| (1 + \delta) \right)^k + \frac{\delta(1 + \delta)}{2\tau}. \end{aligned}$$

This bound is independent of the specific value of j , $1 \leq j \leq m$, but is given in terms of m . We can refine this by examining the j th column of $E_{(k)}$ more closely. Denote the columns of $E_{(k)}$ by

$$E_{(k)} = [\mathbf{e}_1^{(k)} \mathbf{e}_2^{(k)} \dots \mathbf{e}_m^{(k)}].$$

Note that

$$\begin{aligned}
 E_{(k)} &= \Gamma_{p'} E_{(k-1)} (\Gamma_m + \xi_{(k-1)})^{-1} \\
 &= \Gamma_{p'} E_{(k-1)} \Gamma_m^{-1} + \Gamma_{p'} E_{(k-1)} \left((I + \Gamma_m^{-1} \xi_{(k-1)})^{-1} - I \right) \Gamma_m^{-1}, \\
 \|e_j^{(k)}\| &\leq \left| \frac{\gamma_{p+1}}{\gamma_j} \right| \|e_j^{(k-1)}\| + \left| \frac{\gamma_{p+1}}{\gamma_m} \right| \delta e_{\delta, k-1} \\
 &\leq \left| \frac{\gamma_{p+1}}{\gamma_j} \right| \left(\left| \frac{\gamma_{p+1}}{\gamma_j} \right| \|e_j^{(k-2)}\| + \left| \frac{\gamma_{p+1}}{\gamma_m} \right| \delta e_{\delta, k-2} \right) + \left| \frac{\gamma_{p+1}}{\gamma_m} \right| \delta e_{\delta, k-1} \\
 &\leq \left| \frac{\gamma_{p+1}}{\gamma_j} \right|^2 \|e_j^{(k-2)}\| + \delta \left| \frac{\gamma_{p+1}}{\gamma_m} \right|^2 e_{\delta, k-2} + \delta \left| \frac{\gamma_{p+1}}{\gamma_m} \right| e_{\delta, k-1} \text{ as } \left| \frac{\gamma_{p+1}}{\gamma_j} \right| \leq \left| \frac{\gamma_{p+1}}{\gamma_m} \right| \\
 &\leq \dots \dots \dots \\
 &\leq \left| \frac{\gamma_{p+1}}{\gamma_j} \right|^k \|e_j^{(0)}\| + \delta \sum_{\ell=0}^{k-1} \left| \frac{\gamma_{p+1}}{\gamma_m} \right|^{k-\ell} e_{\delta, \ell} \\
 &\leq \left| \frac{\gamma_{p+1}}{\gamma_j} \right|^k \|e_j^{(0)}\| + \alpha \delta \sum_{\ell=0}^{k-1} \left| \frac{\gamma_{p+1}}{\gamma_m} \right|^{k-\ell} \left| \frac{\gamma_{p+1}}{\gamma_m} \right|^\ell (1+\delta)^\ell \\
 &\leq \alpha \left| \frac{\gamma_{p+1}}{\gamma_j} \right|^k + \alpha \delta \left| \frac{\gamma_{p+1}}{\gamma_m} \right|^k \sum_{\ell=0}^{k-1} (1+\delta)^\ell.
 \end{aligned}$$

Therefore, an alternative bound on $\|x_j - s_j\|_B$ is

$$\|x_j - s_j\|_B \leq \alpha \left| \frac{\gamma_{p+1}}{\gamma_j} \right|^k + \alpha \delta \left| \frac{\gamma_{p+1}}{\gamma_m} \right|^k \sum_{\ell=0}^{k-1} (1+\delta)^\ell + \frac{\delta(1+\delta)}{2\tau}.$$

Both bounds apply to $\|(I - P_{(k)})x_j\|_B$ as by definition it is $\min_{s \in \mathcal{Q}_{(k)}} \|x_j - s\|_B$. This completes the proof of Theorem 4.4. \square

Theorems 4.1 shows that for each x_j of the m eigenvectors x_1, x_2, \dots, x_m , its distance to $\mathcal{Q}_{(k)}$ decreases to zero at a rate of $|\gamma_{p+1}/\gamma_j|^k$. Theorem 4.4 shows that the error in applying $\rho(M)$ does not affect the convergence fundamentally. The convergence rate is degraded (very slightly) to $|\gamma_{p+1}/\gamma_m|^k (1+\delta)^k$, and the distance may only decrease down to a certain nonzero threshold, of the order δ that is commensurate with the accuracy of the linear solvers used to compute $\rho(M)Q$. In particular, iterative solvers are suitable for implementing $\rho(M)$.

5. Convergence of eigenvalues and residuals. The previous section shows that if the subspace dimension p in Algorithm FEAST is chosen large enough so that $|\gamma_{p+1}/\gamma_e| \ll 1$, then the generated subspaces $\mathcal{Q}_{(k)} = \text{span}(Y_{(k)}) = \text{span}(Q_{(k)})$ will capture rapidly the eigenvectors x_1, x_2, \dots, x_e . In fact, if $|\gamma_{p+1}/\gamma_m| \ll 1$ for some m , $e < m \leq p$, the subspace will also capture the additional eigenvectors $x_{e+1}, x_{e+2}, \dots, x_m$ very well. This scenario is typical when there are eigenvalues outside of $[\lambda_-, \lambda_+]$ but close to the boundaries. This means that $\gamma_e \approx \gamma_{e+1} \approx \dots \approx \gamma_m$ for some $m > e$. Thus $|\gamma_{p+1}/\gamma_e| \ll 1$ implies $|\gamma_{p+1}/\gamma_m| \ll 1$ as well.

Now to complete the story, we must show how to make use of those subspaces that have presumably captured the wanted eigenvectors, to actually obtain the target eigenpairs (λ_j, x_j) , $j = 1, 2, \dots, e$. Specifically, we show that $m \geq e$ of the p eigenvalues of $\hat{\Lambda}_{(k)}$ converge to $\lambda_1, \lambda_2, \dots, \lambda_m$, as do the corresponding vectors in

$Q_{(k)} = Y \hat{X}_{(k)}$. Consider steps 5–7 of FEAST at a particular iteration. Omitting the subscript k , we have

$$(5.1) \quad \hat{X}^* Y^* A Y \hat{X} = (\hat{X}^* Y^* B Y \hat{X}) \hat{\Lambda} \Rightarrow Q^* A Q = \hat{\Lambda}.$$

Theorems 4.1 and 4.4 show that Q is of the form

$$Q = [(X_m + X_{m'} G) L^{-1} \quad V] U,$$

where G encapsulates the E and F terms: $X_{m'} G = X_{p'} E + X_{m'} F$. Q is B -orthonormal, and U is unitary of dimension $p \times p$. The next lemma analyzes the structure of $\text{span}(Q)$, which is key to the convergence of eigenpairs (Theorem 5.2) and to the useful properties of the \hat{B} and Y matrices (Theorem 5.3).

LEMMA 5.1. Consider an $n \times p$ B -orthonormal matrix Q of the form

$$Q = [(X_m + X_{m'} G) L^{-1} \quad V] U$$

for some $m \leq p$ where $\|G\| = \epsilon \leq 1/2$, V is of dimension $n \times (p-m)$, U is unitary of dimension $p \times p$, and $L^{-1} = [(X_m + X_{m'} G)^* B (X_m + X_{m'} G)]^{-1/2}$. Then we have the following.

- (1) $\|L^{-1} - I_m\| \leq \epsilon^2$. V can be represented as $V = X_m S + X_{m'} H R$, where $\|S\| \leq \epsilon$, H is $(n-m) \times (p-m)$, where $H^* H = I_{p-m}$ and $\|R - I_{p-m}\| \leq \epsilon^2$.
- (2)

$$X^* B Q = \left(\left[\begin{array}{c|c} I_m & \\ \hline & H \end{array} \right] + \Theta \right) U,$$

$$\Theta = \left[\begin{array}{c|c} \Theta_{11} & \Theta_{12} \\ \hline \Theta_{21} & \Theta_{22} \end{array} \right], \quad \Theta_{11} \text{ is } m \times m,$$

$$\|\Theta_{11}\|, \|\Theta_{22}\| \leq \epsilon^2, \|\Theta_{12}\|, \|\Theta_{21}\| \leq (1 + \epsilon^2)\epsilon.$$

- (3) Given any $n \times n$ real diagonal matrix $D = \text{diag}(d_1, d_2, \dots, d_n) = \text{diag}(D_m, D_{m'})$,

$$(Q^* B X) D (X^* B Q) = U^* \left(\left[\begin{array}{c|c} D_m & \\ \hline & H^* D_{m'} H \end{array} \right] + \Delta \right) U,$$

$$\Delta = \left[\begin{array}{c|c} \Delta_{11} & \Delta_{12} \\ \hline \Delta_{12}^* & \Delta_{22} \end{array} \right], \quad \Delta_{11} \text{ is } m \times m,$$

$$\|\Delta_{11}\|, \|\Delta_{22}\| \leq 4\|D\|\epsilon^2, \|\Delta_{12}\| \leq 4\|D\|\epsilon.$$

Proof. Since $L^{-1} = (I_m + G^* G)^{-1/2}$, $\|G^* G\| \leq \epsilon^2 \leq 1/4 \leq 1/2$, Lemma 4.3 shows that $\|L^{-1} - I_m\| \leq \epsilon^2$. Q is B -orthonormal, and so is QU^* as U is a unitary matrix by assumption. Represent V in the basis vectors X_m and $X_{m'}$:

$$V = (X_m X_m^* B + X_{m'} X_{m'}^* B) V = X_m S + X_{m'} T.$$

Note that CV , CX_m , and $CX_{m'}$ have orthonormal columns, and CX_m is orthogonal with $CX_{m'}$. Thus $\|S\|, \|T\| \leq 1$. V being B -orthogonal with the first m columns of QU^* implies $S + G^* T = 0$. Therefore, $\|S\| = \|-G^* T\| \leq \|G^*\| = \epsilon$. $V^* B V = I_{p-m}$ then implies

$$T^* T = I_{p-m} + (-S^* S), \quad \|-S^* S\| \leq \epsilon^2 \leq 1/2.$$

Lemma 4.3 shows that $R \stackrel{\text{def}}{=} (T^*T)^{1/2}$ satisfies $\|R - I_{p-m}\| \leq \epsilon^2$. Clearly, $H \stackrel{\text{def}}{=} TR^{-1}$ leads to $H^*H = I_{p-m}$. Summarizing, $V = X_m S + X_{m'} H R$, $\|S\| \leq \epsilon$, $H^*H = I_{p-m}$, and $\|R - I_{p-m}\| \leq \epsilon^2$. This establishes the first point of the lemma.

Since $Q = [(X_m + X_{m'}G)L^{-1} \quad X_m S + X_{m'} H R] U$,

$$\begin{aligned} X^* B Q &= \begin{bmatrix} L^{-1} & S \\ GL^{-1} & HR \end{bmatrix} U \\ &= \left(\left[\begin{array}{c|c} I_m & \\ \hline & H \end{array} \right] + \begin{bmatrix} L^{-1} - I_m & S \\ GL^{-1} & H(R - I_{p-m}) \end{bmatrix} \right) U \\ &= \left(\left[\begin{array}{c|c} I_m & \\ \hline & H \end{array} \right] + \Theta \right) U, \end{aligned}$$

$\|\Theta_{11}\|, \|\Theta_{22}\| \leq \epsilon^2$, $\|\Theta_{21}\| \leq (1 + \epsilon^2)\epsilon$, $\|\Theta_{12}\| \leq \epsilon \leq (1 + \epsilon^2)\epsilon$. This establishes the second point of the lemma.

Let $D = \text{diag}(D_m, D_{m'})$ be any $n \times n$ real diagonal matrix. Using the structure of $X^* B Q$ just established, we have

$$\begin{aligned} (Q^* B X) D (X^* B Q) &= U^* \left(\left[\begin{array}{c|c} D_m & \\ \hline & H^* D_{m'} H \end{array} \right] + \Theta^* D + D \Theta + \Theta^* D \Theta \right) U \\ &= U^* \left(\left[\begin{array}{c|c} D_m & \\ \hline & H^* D_{m'} H \end{array} \right] + \Delta \right) U. \end{aligned}$$

Bounding Δ in a straightforward manner yields

$$\begin{aligned} \|\Delta_{11}\| &\leq \|D\| (2\epsilon^2 + \epsilon^4 + (1 + \epsilon^2)^2 \epsilon^2) \leq 4\|D\|\epsilon^2, \\ \|\Delta_{22}\| &\leq \|D\| (2\epsilon^2 + \epsilon^4 + \epsilon^2) \leq 4\|D\|\epsilon^2, \\ \|\Delta_{12}\| &\leq \|D\| ((1 + \epsilon^2)^2 \epsilon + (1 + \epsilon^2)\epsilon) \leq 4\|D\|\epsilon, \end{aligned}$$

all making use of the assumption $\epsilon \leq 1/2$. \square

THEOREM 5.2. *Consider an Algorithm FEAST that exhibits subspace convergence as in Theorem 4.4. For any iteration k , $Q_{(k)}$ is represented as in Lemma 5.1,*

$$Q_{(k)} = [(X_m + X_{m'}G_{(k)})L_{(k)}^{-1}, \quad X_m S_{(k)} + X_{m'} H_{(k)} R_{(k)}] U_{(k)}.$$

Denote $\|G_{(k)}\|$ by ϵ_k and define the spectral gap η_k as

$$\eta_k \stackrel{\text{def}}{=} \begin{cases} \min_{\lambda \in \text{eig}(\Lambda_m), \mu \in \text{eig}(H_{(k)}^* \Lambda_{m'} H_{(k)})} |\lambda - \mu| / \|\Lambda\| & \text{if } m < p, \\ \infty & \text{if } m = p. \end{cases}$$

As long as $\epsilon_k \leq 1/2$, there are m eigenpairs $(\hat{\lambda}_j, \hat{x}_j)$ among the p eigenpairs in $(\hat{\Lambda}_{(k)}, \hat{X}_{(k)})$ such that

$$|\lambda_j - \hat{\lambda}_j| \leq 4\|\Lambda\| (\epsilon_k^2 + \min\{\epsilon_k, 4\epsilon_k^2/\eta_k\})$$

and

$$\|A q_j - \hat{\lambda}_j B q_j\| \leq 12\|C\| \|\Lambda\| \epsilon_k (1 + 1/\eta_k).$$

Proof. As displayed in (5.1), $Q_{(k)}^* A Q_{(k)} = \hat{\Lambda}_{(k)}$, so that the eigenvalues of $\hat{\Lambda}_{(k)}$ are those of $Q_{(k)}^* A Q_{(k)}$. Because $A = B X \Lambda X^* B$, Lemma 5.1 shows that

$$\begin{aligned}
Q_{(k)}^* A Q_{(k)} &= (Q_{(k)}^* B X) \Lambda (X B Q_{(k)}) \\
&= U_{(k)}^* (W + \Delta_{\text{off}} + \Delta_{\text{diag}}) U_{(k)}, \\
\text{eig}(Q_{(k)}^* A Q_{(k)}) &= \text{eig}(W + \Delta_{\text{off}} + \Delta_{\text{diag}}),
\end{aligned}$$

where

$$W = \left[\begin{array}{c|c} \Lambda_m & \\ \hline H_{(k)}^* \Lambda_{m'} H_{(k)} & \end{array} \right], \quad \Delta_{\text{off}} = \left[\begin{array}{c|c} & \Delta_{12} \\ \hline \Delta_{12}^* & \end{array} \right], \quad \Delta_{\text{diag}} = \left[\begin{array}{c|c} \Delta_{11} & \\ \hline & \Delta_{22} \end{array} \right],$$

where Δ_{off} and Δ_{diag} are small perturbations: $\|\Delta_{\text{diag}}\| \leq 4\|\Lambda\|\epsilon_k^2$ and $\|\Delta_{\text{off}}\| \leq 4\|\Lambda\|\epsilon_k$. Of the p eigenvalues of W , m of them are $\lambda_1, \lambda_2, \dots, \lambda_m$. We analyze the eigenvalues of $W + \Delta_{\text{off}} + \Delta_{\text{diag}}$ by standard Hermitian perturbation theory (see, for example, [7, 19, 31, 18]). First, there are m eigenvalues $\lambda'_1, \lambda'_2, \dots, \lambda'_m$ of $W + \Delta_{\text{off}}$ such that

$$(5.2) \quad |\lambda_j - \lambda'_j| \leq \min\{\|\Delta_{\text{off}}\|, \|\Delta_{\text{off}}\|^2/(\eta_k \|\Lambda\|)\} \leq 4\|\Lambda\| \min\{\epsilon_k, 4\epsilon_k^2/\eta_k\}.$$

In the case $m = p$, $\Delta_{\text{off}} = 0$, and the definition of $\eta_k = \infty$ correctly reflects that $|\lambda_j - \lambda'_j| = 0$. Next, apply the standard Weyl perturbation theorem on $(W + \Delta_{\text{off}}) + \Delta_{\text{diag}}$, where Δ_{diag} is the perturbation term. There are m eigenvalues $\hat{\lambda}_1, \hat{\lambda}_2, \dots, \hat{\lambda}_m$ of $W + \Delta_{\text{off}} + \Delta_{\text{diag}}$ such that

$$(5.3) \quad |\lambda'_j - \hat{\lambda}_j| \leq \|\Delta_{\text{diag}}\| \leq 4\|\Lambda\|\epsilon_k^2.$$

Combining (5.2) and (5.3) gives

$$|\lambda_j - \hat{\lambda}_j| \leq 4\|\Lambda\| (\epsilon_k^2 + \min\{\epsilon_k, 4\epsilon_k^2/\eta_k\}).$$

Moving on to examine the residual of the approximate eigenvector \mathbf{q}_j , note that

$$\mathbf{q}_j = [(X_m + X_{m'} G_{(k)}), L_{(k)}^{-1}, \quad X_m S_{(k)} + X_{m'} H_{(k)} R_{(k)}] \mathbf{u}_j,$$

\mathbf{u}_j being the j th column of $U_{(k)}$. Then

$$\begin{aligned}
Q_{(k)}^* A Q_{(k)} - \hat{\Lambda} = 0 &\implies U_{(k)}^* (W + \Delta_{\text{off}} + \Delta_{\text{diag}}) U_{(k)} - \hat{\Lambda} = 0 \\
&\implies (W + \Delta_{\text{off}} + \Delta_{\text{diag}}) \mathbf{u}_j - \hat{\lambda}_j \mathbf{u}_j = 0 \\
&\implies \|W \mathbf{u}_j - \hat{\lambda}_j \mathbf{u}_j\| \leq 4\|\Lambda\|\epsilon_k(1 + \epsilon_k).
\end{aligned}$$

Partition \mathbf{u}_j into its top m and bottom $p - m$ elements, $\mathbf{u}_j = \begin{bmatrix} \mathbf{u}_j^{(t)} \\ \mathbf{u}_j^{(b)} \end{bmatrix}$, we see that

$$\eta_k \|\Lambda\| \|\mathbf{u}_j^{(b)}\| \leq \|H_{(k)}^* \Lambda_{m'} H_{(k)} \mathbf{u}_j^{(b)} - \hat{\lambda}_j \mathbf{u}_j^{(b)}\| \leq 4\|\Lambda\|\epsilon_k(1 + \epsilon_k).$$

Thus $\|\mathbf{u}_j^{(b)}\| \leq 4\epsilon_k(1 + \epsilon_k)/\eta_k$. Furthermore,

$$\|(\Lambda_m - \hat{\lambda}_j I) \mathbf{u}_j^{(t)}\| \leq 4\|\Lambda\|\epsilon_k(1 + \epsilon_k).$$

By estimating the residual, we have

$$\begin{aligned}
A\mathbf{q}_j &= A[(X_m + X_{m'}G_{(k)})L_{(k)}^{-1}, V_{(k)}]\mathbf{u}_j \\
&= (BX \wedge X^*B)[(X_m + X_{m'}G_{(k)})L_{(k)}^{-1}, V_{(k)}]\mathbf{u}_j \\
&= B\left((X_m\Lambda_m + X_{m'}\Lambda_{m'}G_{(k)})L_{(k)}^{-1}\mathbf{u}_j^{(t)} + X\Lambda(X^*BV_{(k)})\mathbf{u}_j^{(b)}\right), \\
\widehat{\lambda}_j B\mathbf{q}_j &= B\left(\widehat{\lambda}_j(X_m + X_{m'}G_{(k)})L_{(k)}^{-1}\mathbf{u}_j^{(t)} + \widehat{\lambda}_j V_{(k)}\mathbf{u}_j^{(b)}\right), \\
A\mathbf{q}_j - \widehat{\lambda}_j B\mathbf{q}_j &= B\left(X_m(\Lambda_m - \widehat{\lambda}_j I)L_{(k)}^{-1}\mathbf{u}_j^{(t)} + X_{m'}(\Lambda_{m'} - \widehat{\lambda}_j I)G_{(k)}L_{(k)}^{-1}\mathbf{u}_j^{(t)}\right. \\
&\quad \left.+ (X\Lambda(X^*BV_{(k)}) - \widehat{\lambda}_j V_{(k)})\mathbf{u}_j^{(b)}\right), \\
&= C^*\left(CX_m(\Lambda_m - \widehat{\lambda}_j I)L_{(k)}^{-1}\mathbf{u}_j^{(t)} + CX_{m'}(\Lambda_{m'} - \widehat{\lambda}_j I)G_{(k)}L_{(k)}^{-1}\mathbf{u}_j^{(t)}\right. \\
&\quad \left.+ (CX\Lambda(X^*BV_{(k)}) - \widehat{\lambda}_j CV_{(k)})\mathbf{u}_j^{(b)}\right).
\end{aligned}$$

Note that $\|CX_m\|$, $\|CX_{m'}\|$, $\|CX\|$, and $\|X^*BV\|$ are all of unity as CX is unitary and V is B -orthonormal. Estimating $\|\Lambda_{m'} - \widehat{\lambda}_j I\| \leq 2\|\Lambda\|$ and using bounds of $\|L_{(k)}^{-1}\|$ and $\mathbf{u}_j^{(b)}$, we have

$$\begin{aligned}
\|A\mathbf{q}_j - \widehat{\lambda}_j B\mathbf{q}_j\| &\leq \|C\|\|\Lambda\| (4\epsilon_k(1 + \epsilon_k)(1 + \epsilon_k^2) + 2\epsilon_k(1 + \epsilon_k^2) + 8\epsilon_k(1 + \epsilon_k)/\eta_k), \\
&\leq 12\|C\|\|\Lambda\|\epsilon_k(1 + 1/\eta_k),
\end{aligned}$$

using $\epsilon_k \leq 1/2$. This completes the proof. \square

Theorem 5.2 shows that if the subspace dimension p is large enough, we would expect that some m , $m \geq e$, eigenvalues among the p values of $\widehat{\Lambda}_{(k)}$ converge to the actual eigenvalues of $AX = BX\Lambda$. Furthermore, e of these eigenvalues are inside $\mathcal{I} = [\lambda_-, \lambda_+]$. If the spectral gaps η_k are never too small, the convergence rate of eigenvalues is essentially $|\gamma_{p+1}/\gamma_m|^{2k}$ while the residual vector norms $\|A\mathbf{q}_j - \widehat{\lambda}_j B\mathbf{q}_j\|$ decrease at the rate $|\gamma_{p+1}/\gamma_m|^k$.

However, all we can conclude about the remaining $p-m$ eigenvalues (when $m < p$) is that they are close to the eigenvalues of $H_{(k)}^* \Lambda_{m'} H_{(k)}$, which can change at each iteration. As $H_{(k)}$ has orthonormal columns, each of these $p-m$ eigenvalues, $\mu \in \text{eig}(H_{(k)}^* \Lambda_{m'} H_{(k)})$, satisfies $\min_{j>m} \lambda_j \leq \mu \leq \max_{j>m} \lambda_j$. In particular, some or all of them can fall inside \mathcal{I} . Hence there may be more than e eigenvalues of $\widehat{\Lambda}_{(k)}$ that fall inside \mathcal{I} . Our general experience is that, a posteriori, exactly e of the eigenvalues of $\widehat{\Lambda}_{(k)}$ fall inside \mathcal{I} . Nevertheless, knowing the value of e , a priori, can be exploited to help monitor convergence. It turns out that the value e can be accurately estimated as a by-product of Algorithm FEAST. Theorem 5.3 shows that the distribution of $\widehat{B}_{(k)}$'s eigenvalues offers a good estimate of e . More importantly, this distribution gives us an indication if the choice of p is too small. Due to the nature of $\rho(M)$, $p < e$ would in general lead to nonconvergence of FEAST. For example, consider $Q_{(0)} = X_e W$, where W is $e \times p$, $p < e$, and $W^*W = I_p$. Suppose $\rho(M)$ is the exact spectral projector, $\rho(M) = X_e X_e^*$. Let W^*AW have the spectral decomposition VDV^* . Algorithm FEAST will simply get stuck after the first iteration at $Q_{(k)} = X_e W V$ and $\widehat{\Lambda}_{(k)} = D$. The key reason is that by design $\rho(M)$ maps all the possibly distinct eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_e$ to almost identically 1. We note that nonconvergence due to $p < e$ was observed in Experiment 3.1 of [15].

THEOREM 5.3. Consider an Algorithm FEAST that exhibits subspace convergence as in Theorem 4.4. For any iteration k , $Q_{(k)}$ is represented as in Lemma 5.1,

$$Q_{(k)} = [(X_m + X_{m'} G_{(k)}) L_{(k)}^{-1}, \quad X_m S_{(k)} + X_{m'} H_{(k)} R_{(k)}] U_{(k)},$$

where $\|G_{(k)}\| = \epsilon_k$ is small. The eigenvalues of $\hat{B}_{(k+1)}$ are close to those of the matrix $\text{diag}(\Gamma_m^2, H_{(k)}^* \Gamma_{m'}^2 H_{(k)})$. The eigenvalues of $Z \stackrel{\text{def}}{=} Q_{(k)}^* B Y_{(k+1)}$ are close to those of $\text{diag}(\Gamma_m, H_{(k)}^* \Gamma_{m'} H_{(k)})$. In particular, the number e of target eigenvalues in $[\lambda_-, \lambda_+]$ can be estimated by the number of $\hat{B}_{(k+1)}$'s eigenvalues that are no less than $1/4$, or the number of Z 's eigenvalues no less than $1/2$.

Proof. Given

$$Q_{(k)} = [(X_m + X_{m'} G_{(k)}) L_{(k)}^{-1}, \quad X_m S_{(k)} + X_{m'} H_{(k)} R_{(k)}] U_{(k)},$$

we see that

$$\begin{aligned} \hat{B}_{(k+1)} &= Y_{(k+1)}^* B Y_{(k+1)} \\ &= Q_{(k)}^* \rho^*(M) B \rho(M) Q_{(k)} \\ &= (Q_{(k)}^* B X) \Gamma X^* B X \Gamma (X^* B Q_{(k)}) \quad \text{because } \rho(M) = X \Gamma X^* B \\ &= (Q_{(k)}^* B X) \Gamma^2 (X^* B Q_{(k)}) \\ &= U_{(k)}^* \left(\text{diag}(\Gamma_m^2, H_{(k)}^* \Gamma_{m'}^2 H_{(k)}) + \Delta \right) U_{(k)} \quad \text{by Lemma 5.1.} \end{aligned}$$

Clearly, the eigenvalues of $\hat{B}_{(k+1)}$ are close to those of $\text{diag}(\Gamma_m^2, H_{(k)}^* \Gamma_{m'}^2 H_{(k)})$. Similarly,

$$\begin{aligned} Z &= Q_{(k)}^* B Y_{(k+1)} \\ &= (Q_{(k)}^* B X) \Gamma (X^* B Q_{(k)}) \\ &= U_{(k)}^* \left(\text{diag}(\Gamma_m, H_{(k)}^* \Gamma_{m'} H_{(k)}) + \Delta \right) U_{(k)} \quad \text{by Lemma 5.1.} \end{aligned}$$

Note, however, that $\gamma_1 \geq \dots \geq \gamma_e \geq 1/2 > |\gamma_{e+1}| \geq \dots \geq |\gamma_n|$ and

$$\min_{j > m'} \gamma_j^2 \leq \text{eig}(H_{(k)}^* \Gamma_{m'}^2 H_{(k)}) \leq \max_{j > m'} \gamma_j^2$$

because $H_{(k)}$ has orthonormal columns. For small $\|G_{(k)}\|$, the number of $\hat{B}_{(k+1)}$'s eigenvalues that are no smaller than $1/4$ is an accurate estimate of e . Similar arguments show that the number e can be estimated by counting the eigenvalues of Z that are no less than $1/2$. \square

Let us elaborate on a number of details related to FEAST now that all the main theoretical properties have been presented.

1. The algorithm requires a choice of the subspace dimension, p . If the user has an educated guess of e , the actual number of eigenvalues in the search interval, p can be set to be about 1.5 times that. Otherwise, a somewhat arbitrary choice is set. The following discussions are germane.
 - Whenever $p \geq e$, convergence is possible and the rate is generally determined by $|\gamma_{p+1}/\gamma_e|$. Tables 3–6 of section 6 are illustrations. The examples there exhibit rates consistent with $|\gamma_{p+1}/\gamma_e|$. Theoretically, $p = e$ does not lead to nonconvergence. Nevertheless, in practice $|\gamma_{p+1}/\gamma_e| = |\gamma_{e+1}/\gamma_e|$ will be close to 1, rendering convergence slow. This slow convergence was observed in Experiment 3.1 of [15].

- In general, a choice of $p \geq e$, where $|\gamma_{p+1}/\gamma_e| \ll 1$, is desirable as it leads to fast convergence. As shown in Theorem 4.1, as long as $|\gamma_p| > 0$ and $X^*BQ_{(0)}$ has full column rank, $\rho(M)Q_{(k)}$ is of full rank p for all iterations k . Note that $\rho(M)$ is not the exact spectral projector and is theoretically almost always invertible. This is because $\rho(\mu)$ is a rational function and has only a small number of zeros on the real line (see section 3.3). So in all likelihood $\rho(\Lambda)$ is invertible. However, $\rho(\mu)$ decays rapidly, so from a numerical point of view, $\rho(M)$ could be numerically rank deficient if p is chosen too large,¹ for example, $p \geq 4e$. Consequently, $Y_{(1)} = \rho(M)Q_{(0)}$ will be rank deficient, leading to a semi-definite $\hat{B}_{(1)}$. The conservative precautionary approach is to perform an SVD or a rank-revealing QR factorization [8, 11] on $Y_{(1)}$ to possibly reduce the value of p before proceeding further. However, we found that the greedy approach of letting LAPACK's Cholesky factorization on $\hat{B}_{(1)}$ proceed naturally works very well in practice. If the factorization fails at the K th column, we reset $p \leftarrow K - 1$ and use these first p columns of $Y_{(1)}$. That this strategy is effective has to do with the randomness of $Q_{(0)}$. While $\rho(M)$ is numerically rank deficient (of low rank), each $\rho(M)q_j$ is a random mixture of all the columns of $\rho(M)$. QR without column pivoting on such a $\rho(M)Q_{(0)}$ is an effective “greedy” rank-revealing algorithm. The review article [9] and references thereof contain much information about recent works on randomized algorithms.
 - If $p < e$, then as discussed previously, FEAST in general will fail to converge. If $p \geq e$ but $|\gamma_{p+1}/\gamma_e|$ close to unity, convergence will be slow. We exploit Theorem 5.3 to protect against both scenarios. In practice, we compute the eigenvalues of $\hat{B}_{(2)}$. If the minimum eigenvalue is bigger than threshold/4 for some “threshold” less than 1, for example, 1/10, we warn against p being set too small. For p not considered too small, our experience has been that the count of $\hat{B}_{(2)}$'s eigenvalues is not smaller than 1/4 to match e , the number of eigenvalues in the search interval.
2. The search interval $\mathcal{I} = [\lambda_-, \lambda_+]$.
- This is an obvious feature for parallelism. One would be able to locate the eigenvalues and eigenvectors within different search intervals independently and simultaneously. The convergence theory established here shows that as long as $|\gamma_{p+1}/\gamma_e|$ is suitably small, eigenvalues within each search interval can be obtained, each with an eigenvector that results in a small residual. (See Theorem 5.2 for detailed conditions.) Computed eigenvectors within one search interval are mutually B -orthogonal (assuming an accurate eigensolver is used for the reduced problem).
 - A natural application of the previous point is to partition one search interval $\mathcal{I} = [\lambda_-, \lambda_+]$ into a sequence of connecting intervals $\mathcal{I}^{(k)} = [\lambda^{(k-1)}, \lambda^{(k)}]$, $k = 1, 2, \dots, K$, where $\lambda_- = \lambda^{(0)} < \lambda^{(1)} < \dots < \lambda^{(K)} = \lambda_+$. Each $\mathcal{I}^{(k)}$ is tackled independently. Convergence theory applies on each subinterval. However, in the case when there is a cluster of eigenvalues around a break point, say $\lambda^{(k)}$, there will be a natural loss of B -orthogonality between the computed eigenvectors associated to the clusters on the left interval $\mathcal{I}^{(k)} = [\lambda^{(k-1)}, \lambda^{(k)}]$ and to those on the right

¹What makes p too large is obviously dependent upon the actual distribution of the eigenvalues of the problem in question.

$\mathcal{I}^{(k+1)} = [\lambda^{(k)}, \lambda^{(k+1)}]$. This phenomenon is due to the sensitivity of eigenvectors associated with a cluster of eigenvalues (see [6, section 5.2], for example). But Algorithm FEAST offers a natural strategy to handle this situation. If there is indeed a cluster of eigenvalues around one of the points of a search interval and if FEAST is indeed converging at a reasonable rate, then p must have already been chosen large enough to include the number of eigenvalues in the cluster (including those outside of the search interval). Thus in the end, the computations for $\mathcal{I}^{(k)}$ and $\mathcal{I}^{(k+1)}$ will each have obtained all the clustered eigenvalues and a complete set of B -orthonormal eigenvectors. It suffices to adopt one of these two set of eigenvectors. Section 6.4 illustrates this idea.

3. Convergence criteria.

- The original implementation, FEAST Version 1.0, only monitors convergence of eigenvalues and does so through the surrogate of “trace,” namely the sum of all the computed eigenvalues $\hat{\Lambda}_{(k)}$ that fall inside \mathcal{I} . Our analysis exposes two shortcomings of this strategy. First, eigenvalues in general converge faster than the residual norms. Thus the algorithm may terminate before the residual norms are driven down to as small a level as is achievable. Second, it is possible that some of $\hat{\Lambda}_{(k)}$ ’s eigenvalues are “spurious.” These spurious eigenvalues generally do not converge, and monitoring them will only defeat FEAST’s convergence test, resulting in a false negative.
- FEAST Version 2.1 [23] corrected both problems. First, it offers the user an option to set convergence thresholds for either eigenvalues or residuals. Second, with the estimator of e , the actual number of eigenvalues inside the search interval \mathcal{I} , the absence of spurious eigenvalues is easily recognized. When the presence of spurious eigenvalues is detected, they are identified with the help of residual norms. The trace consists of the sum of computed eigenvalues without the spurious ones. Convergence of eigenvalues is monitored by the surrogate $|\text{trace}_{(k-1)} - \text{trace}_{(k)}| / \max\{|\lambda_-|, |\lambda_+|\}$.

FEAST Version 2.1 [23] incorporated these improvements and is outlined as *Algorithm FEAST with estimate*.

6. Numerical experiments. The original FEAST paper [21] demonstrated that the algorithm converges in practice on a number of large sparse matrices that arise from applications. Direct as well as iterative solvers were used in the examples there. The purpose here is to scrutinize the various numerical properties as well as subtleties discussed in the previous sections. To this end, we therefore utilize primarily synthetic, controlled, examples. Given the problem dimension n and a search interval $[\lambda_-, \lambda_+]$, we generate Λ , the diagonal matrix containing the eigenvalues, somewhat randomly, except for special placements of some of the eigenvalues near the boundaries of $[\lambda_-, \lambda_+]$. Random unitary matrices are the basic ingredient of our test matrices. With a specified condition number κ , random matrix C is generated as $U\Sigma V^*$, where U and V are random unitary matrices and Σ are random singular values so as to make the condition number of C equal κ . The matrix B is constructed as $B = C^*C$. The eigenvectors X are constructed by solving $CX = W$, where W is a random unitary matrix. Finally, the matrix A is constructed as $A = (BX)\Lambda(BX)^*$. This way,

$$AX = BX\Lambda,$$

and (X, Λ) is the solution to the generalized eigenproblem defined by A and B .

Algorithm FEAST with estimate.

-
- 1: Specify $\mathcal{I} = [\lambda_-, \lambda_+]$ and a Gauss–Legendre quadrature choice of q .
 - 2: Pick p and p random n -vectors $Q_{(0)} = [q_1, q_2, \dots, q_p]$. Set $k \leftarrow 1$.
 - 3: **repeat**
 - 4: Approximate subspace projection (see (3.7)): $Y_{(k)} \leftarrow \rho(M) \cdot Q_{(k-1)}$.
 - 5: Form reduced system: $\hat{A}_{(k)} \leftarrow Y_{(k)}^* A Y_{(k)}$, $\hat{B}_{(k)} \leftarrow Y_{(k)}^* B Y_{(k)}$.
 - 6: **if** $k = 2$ **then**
 - 7: Compute $\hat{B}_{(k)}$'s p eigenvalues.
 - 8: If minimum eigenvalue $\geq \text{thres}/4$, report that p is probably too small.
 - 9: (Note: $\text{thres} \leq 1$. FEAST Version 2.1 uses $\text{thres} = 1$.)
 - 10: Otherwise, set \hat{e} to be number of eigenvalues $\geq 1/4$ (\hat{e} estimates e).
 - 11: **end if**
 - 12: Solve p -dimension eigenproblem: $\hat{A}_{(k)} \hat{X}_{(k)} = \hat{B}_{(k)} \hat{X}_{(k)} \hat{\Lambda}_{(k)}$ for $\hat{\Lambda}_{(k)}$, $\hat{X}_{(k)}$.
 - 13: **if** $k = 1$ and the above fails due to nondefinite $\hat{B}_{(1)}$ **then**
 - 14: Reduce p to the last column of $\hat{B}_{(1)}$ before Cholesky fails.
 - 15: **end if**
 - 16: Set $Q_{(k)} \leftarrow Y_{(k)} \hat{X}_{(k)}$, in particular $Q_{(k)}^* B Q_{(k)} = I_p$.
 - 17: $k \leftarrow k + 1$.
 - 18: **until** Stopping criteria based on the \hat{e} smallest residuals or trace of \hat{e} computed eigenvalues
-

6.1. Approximate spectral projector via quadrature. A crucial property of the quadrature-based approximate spectral projector $\rho(M)$ is that it preserves M 's eigenvectors, $M = B^{-1}A$, and changes only its eigenvalues from Λ to $\Gamma = \rho(\Lambda)$ (see (3.8) and (3.9)):

$$\rho(M) \stackrel{\text{def}}{=} \sum_{k=1}^K \sigma_k (\gamma_k B - A)^{-1} \cdot B = X \rho(\Lambda) X^* B = X \rho(\Lambda) X^{-1}.$$

We generate matrices A, B, Λ, X (as outlined previously) of dimension $n = 300$ with the elements of Λ to be uniformly distributed in $[-30, 30]$. The C matrices used in generating $B = C^*C$ have condition number 100. We used the Gauss–Legendre quadrature rule with 6, 8, and 10 quadrature points on $[-1, 1]$. For each test system and quadrature rule, we compute

$$\epsilon \stackrel{\text{def}}{=} \max_{1 \leq j \leq n} \frac{\|e_j\|}{\|M\|}, \quad e_j = \rho(M)x_j - \rho(\lambda_j)x_j.$$

For each quadrature rule, 200 test cases are generated; Table 2 tabulates the maximum, mean, and standard deviation of these 200 ϵ s.

6.2. Convergence of subspace iteration using approximate spectral projector. To illustrate Theorem 4.1, we generate a complex generalized problem of dimension $n = 500$. We use Gauss–Legendre quadrature with eight points on $[-1, 1]$. $[\lambda_-, \lambda_+]$ is set to $[15, 17]$. The n eigenvalues are generated as follows. We pick four eigenvalues in $[15, 17]$ by picking three randomly with uniform distribution in the region $[15.2, 16.8]$. The fourth is set to be 17. This guarantees that $|\rho(\lambda_j)| \approx 1$ for $j = 1, 2, 3$, and $|\rho(\lambda_4)| = 1/2$. These four eigenvalues are the only ones in $[15, 17]$ and hence $e = 4$. Next, five eigenvalues are set to be in the interval $(17, 18]$ such that

TABLE 2

Key property of quadrature-based approximate spectral projector. For each eigenpair $(\lambda_j, \mathbf{x}_j)$ of M , we check whether, indeed, $\rho(M)\mathbf{x}_j \approx \rho(\lambda_j)\mathbf{x}_j$.

Statistics of $\{\ \rho(M)\mathbf{x}_j - \rho(\lambda_j)\mathbf{x}_j\ /\ M\ \}$	Quadrature points of Gauss–Legendre		
	6	8	10
Maximum	5.5×10^{-15}	9.0×10^{-15}	1.0×10^{-14}
Mean	2.1×10^{-16}	2.4×10^{-16}	2.9×10^{-16}
Standard deviation	5.5×10^{-16}	8.0×10^{-16}	9.8×10^{-16}

the values of $|\rho(\lambda_j)|$ are $2^{-\ell}$ for $\ell = 3, 5, 7, 9, 11$. The remaining 491 eigenvalues are chosen randomly with uniform distribution on the set $[-40, 14] \cup [18, 60]$. The iteration of *Algorithm subspace iteration* is carried out with $p = 8$. With this choice of p , $|\gamma_{p+1}/\gamma_j|$ is 2^{-11} for $j = 1, 2, 3$, and 2^{-10} , 2^{-8} , up to 2^{-2} for the next five eigenvalues. Since the problem is generated, the eigenvectors \mathbf{x}_j are known, and the projectors $P_{(k)} = Q_{(k)}Q_{(k)}^*B$ are easy to compute. We examine the quantities $\|(I - P_{(k)})\mathbf{x}_j\|_B$ for each of $j = 1, 2, \dots, 8$ for five iterations $k = 1, 2, \dots, 5$. Indeed, these norms decrease in a way consistent with what the theorem predicts, except when the ultimate threshold of machine precision is reached. Table 3 tabulates the result.

TABLE 3

Subspace convergence, complex GHEP. $\|(I - P_{(k)})\mathbf{x}_j\|_B$ measures the distance from \mathbf{x}_j to the subspace at the k th iteration. The j th row of the table shows that this distance converges to zero at the rate $|\gamma_p/\gamma_j|^k$. This test problem is designed with $p = 8$ and $\gamma_{p+1} = 2^{-11}$. There are four eigenvalues in $[\lambda_-, \lambda_+] = [15, 17]$. Note that the convergence rates of all the four targets are quite uniform, a signature of the accelerator based on an approximate spectral projector.

j	$\log_2 \left \frac{\gamma_9}{\gamma_j} \right $	$\log_2 \ (I - P_{(k)})\mathbf{x}_j\ _B$ at iterations k				
		$k = 1$	$k = 2$	$k = 3$	$k = 4$	$k = 5$
1	-11	-12.9	-23.8	-34.7	-43.3	-43.2
2	-11	-12.0	-22.8	-33.8	-43.3	-43.3
3	-11	-11.6	-22.4	-33.4	-43.4	-43.4
4	-10	-12.7	-22.6	-32.5	-41.2	-41.1
5	-8	-7.3	-15.1	-23.1	-31.1	-38.5
6	-6	-5.0	-10.8	-16.8	-22.8	-28.8
7	-4	-3.2	-7.0	-11.0	-15.0	-19.8
8	-2	-1.1	-3.0	-5.0	-6.9	-8.9

To illustrate Theorem 4.4, we repeat the same experimental setting except that we have added artificial errors to the linear solvers. To every solution \mathbf{z} of an equation of the form of (3.7):

$$\sigma_k(\phi_k B - A)\mathbf{z} = B\mathbf{q},$$

we modify \mathbf{z} by a random error of $2^{15}u$, u being the machine precision,

$$\mathbf{z} \leftarrow \mathbf{z} + 2^{15}u \|\mathbf{z}\| \Delta,$$

where each element of the n -vector Δ is uniformly random in $[-1/2, 1/2]$. According to the bound of Theorem 4.4, which we restate here (see section 4 for details),

$$\|\mathbf{s}_j - \mathbf{x}_j\|_B \leq \alpha \left| \frac{\gamma_{p+1}}{\gamma_j} \right|^k + \alpha \delta \left| \frac{\gamma_{p+1}}{\gamma_m} \right|^k \sum_{\ell=0}^{k-1} (1 + \delta)^\ell + \frac{\delta(1 + \delta)}{2\tau},$$

where $\delta \approx 2^{15}u$ in our case here. We expect the overall convergence rate to not be affected. The ultimate accuracy limit is degraded commensurate with the artificial errors injected here. The parameter m is flexible. Thus for each eigenvalues λ_j , we can apply the bound with $m = j$. The bound suggests that the actual convergence limit is affected by the last term with the factor $1/|\gamma_m|$. Table 4 is consistent with these predictions. We note that the data in Experiment 3.3 of [15] is consistent with Theorems 4.4 and 5.2.

TABLE 4

Subspace convergence with errors in linear system solutions. Despite errors injected into the solutions of linear systems, the convergence rate of $\|(I - P_{(k)})\mathbf{x}_j\|_B$, which measures the distance between \mathbf{x}_j and the k th subspace, remains unaffected at $|\gamma_p/\gamma_j|^k$. The ultimate accuracy achieved is consistent with the error bound of Theorem 4.4. By iteration 8, the generated subspaces have captured the best they ever can the eigenvectors 1 to 7. The ultimate achievable accuracy degrades by a factor of 2 from eigenvectors 3 to 7, consistent with the factor of $1/|\gamma_j|$, $j = 3, \dots, 7$.

j	$\log_2 \left \frac{\gamma_9}{\gamma_j} \right $	$\log_2 \ (I - P_{(k)})\mathbf{x}_j\ _B$ at iteration k							
		$k = 2$	$k = 3$	$k = 4$	$k = 5$	$k = 6$	$k = 7$	$k = 8$	$k = 9$
1	-11	-21.35	-32.34	-34.39	-34.50	-34.40	-34.46	-34.36	-34.34
2	-11	-22.97	-33.66	-34.34	-34.38	-34.33	-34.37	-34.33	-34.38
3	-11	-23.04	-33.68	-34.37	-34.35	-34.38	-34.42	-34.44	-34.29
4	-10	-19.51	-29.51	-33.40	-33.35	-33.39	-33.44	-33.39	-33.40
5	-8	-16.22	-24.22	-31.17	-31.38	-31.31	-31.39	-31.36	-31.32
6	-6	-12.20	-18.21	-24.21	-29.16	-29.31	-29.43	-29.45	-29.34
7	-4	-7.48	-11.48	-15.49	-19.49	-23.49	-26.96	-27.36	-27.36
8	-2	-5.02	-7.02	-9.01	-11.01	-13.01	-15.00	-17.00	-19.00

6.3. Eigenvalue and residual norm convergence. We illustrate important aspects of Algorithm FEAST as stated in Theorem 5.2. The first example is complex GHEP, dimension 500, with $[\lambda_-, \lambda_+] = [15, 17]$. We generate $e = 5$ eigenvalues well inside this interval. Eigenvalues outside of $[15, 17]$ are generated randomly except for a few specially placed so that $\gamma = 2^{-3, -5, -7, -9}$. Had p been set to $5 = e$, the convergence rate would be somewhat slow. With p set to 8, the convergence rate for the target eigenpairs will be linear with a factor of 2^{-9} . The implication is that the three “collateral” pairs will also converge, except at a slower rate. This example reflects a typical scenario according to our experience with actual applications. There are often eigenvalues outside but quite close to the boundaries of $[\lambda_-, \lambda_+]$. As a result, the successful p will be strictly bigger than e and the iterations will also obtain extra eigenpairs that can be called “collaterals.” Table 5 shows the numerical details. The ratios are $|\gamma_{p+1}/\gamma_j| = 2^{-9}$ for the target eigenpairs. Note that eigenvalue accuracies improve by 2^{-18} per iteration as suggested by Theorem 5.2. This is typical, especially when the collaterals converge. In this event, unless the gap between the target and collateral eigenvalues is small, Theorem 5.2 predicts linear convergence of eigenvalues with the factor $(\gamma_{p+1}/\gamma_j)^2$.

The next example underlines the fact that $p \geq e$ suffices for convergence, in particular for the case $p = e$. We generated two GHEP, each of dimension 500 and $[\lambda_-, \lambda_+] = [15, 17]$. We place five eigenvalues in the interior, and 490 eigenvalues well separated from $[\lambda_-, \lambda_+]$. In the first test case, we place a cluster of five eigenvalues around the point μ where $\rho(\mu) = 2^{-3}$, and in the second case, around μ such that $\rho(\mu) = 2^{-7}$. We set $p = 5$ for both problems. Table 6 shows convergence for both cases at rates that correspond to the two different gaps. Along the same lines, a setting of $p = e$ will result in slow convergence in practice as $|\gamma_{p+1}/\gamma_e| = |\gamma_{e+1}/\gamma_e|$ and

TABLE 5

Convergence of eigenvalues and residual vectors. This table represents a typical scenario. Subspace dimension p is bigger than e but the “extra” dimensions also capture additional invariant subspaces, albeit slower. Note the eigenvalues converge linearly at the rate of $(\gamma_9/\gamma_j)^2$, while residuals do so at that of $|\gamma_9/\gamma_j|$.

j	$\log_2 \left \frac{\gamma_9}{\gamma_j} \right $	Convergence of eigenvalues and residuals							
		$\log_2 \left(\lambda_j - \tilde{\lambda}_j / \ M\ \right)$				$\log_2 \left(\ A\tilde{x}_j - \tilde{\lambda}_j B\tilde{x}_j\ / \ M\ \right)$			
		at iteration k				at iteration k			
		$k = 1$	$k = 2$	$k = 3$		$k = 2$	$k = 3$	$k = 4$	$k = 5$
1	-9	-33.74	-51.15	-64.04		-28.57	-37.56	-46.57	-52.93
2	-9	-32.07	-49.50	-62.32		-27.83	-36.82	-45.83	-52.95
3	-9	-34.40	-51.88	-61.90		-29.23	-38.22	-47.22	-53.15
4	-9	-36.59	-54.23	-62.11		-30.46	-39.46	-48.46	-53.14
5	-9	-34.79	-52.18	-61.23		-29.58	-38.57	-47.58	-52.88
above are e target eigenvalues; below are “collaterals”									
6	-6	-30.73	-40.64	-52.61		-24.92	-30.91	-36.91	-42.91
7	-4	-24.27	-30.73	-38.74		-20.03	-24.04	-28.05	-32.06
8	-2	-24.55	-28.95	-32.99		-19.96	-22.08	-24.08	-26.09

TABLE 6

Convergence of eigenvalues and residual vectors. This table demonstrates convergence when $p = e$. Rate is fundamentally determined by the gap $|\gamma_{p+1}/\gamma_e|$. The two test problems here illustrate different convergence rates due to different gaps. In practice, however, $p = e$ will likely result in slow convergence unless all eigenvalues outside of the search interval $\mathcal{I} = [\lambda_-, \lambda_+]$ are far from it.

j	$\log_2 \left \frac{\gamma_6}{\gamma_j} \right $	Convergence of eigenvalues and residuals							
		$\log_2 \left(\lambda_j - \tilde{\lambda}_j / \ M\ \right)$				$\log_2 \left(\ A\tilde{x}_j - \tilde{\lambda}_j B\tilde{x}_j\ / \ M\ \right)$			
		at iteration k				at iteration k			
		$k = 1$	$k = 2$	$k = 3$	$k = 4$	$k = 3$	$k = 4$	$k = 5$	$k = 6$
1	-3	-14.18	-20.03	-26.04	-32.05	-12.79	-15.80	-18.80	-21.80
2	-3	-11.99	-17.74	-23.75	-29.76	-11.71	-14.71	-17.72	-20.72
3	-3	-13.68	-20.77	-26.79	-32.80	-13.23	-16.25	-19.25	-22.26
4	-3	-14.29	-20.42	-26.43	-32.44	-13.13	-16.14	-19.14	-22.15
5	-3	-14.61	-20.67	-26.68	-32.68	-13.45	-16.46	-19.46	-22.47
above and below are two problems, each with five eigenvalues in \mathcal{I} . The “gaps” $ \gamma_6/\gamma_5 $ are different									
1	-7	-15.65	-29.64	-43.63	-51.58	-24.43	-31.43	-38.42	-45.41
2	-7	-17.52	-31.50	-45.49	-50.99	-25.53	-32.53	-39.53	-46.50
3	-7	-14.95	-28.92	-42.91	-50.58	-24.34	-31.34	-38.34	-45.33
4	-7	-16.03	-30.02	-44.02	-51.32	-25.04	-32.04	-39.03	-46.01
5	-7	-15.19	-29.18	-43.17	-50.58	-24.79	-31.78	-38.78	-45.77

will likely be close to unity. This observation is consistent with the slow convergence observed for $p = e$ in Figure 2 of [15].

The second example is similar to the first: complex GHEP, dimension 500. We generate $e = 5$ eigenvalues well inside this interval. Eigenvalues outside of $[15, 17]$ are generated randomly except for five that are specially placed. One is placed so that $\gamma = 2^{-9}$, and the four others are placed so that γ is strictly bigger than, but extremely close to, 2^{-9} . The other 491 eigenvalues are random but at least 0.5 away from $[15, 17]$. By setting $p = 9$, the convergence rate of the target eigenvalues is expected to be linear with a factor $(2^{-9})^2 = 2^{-18}$ or smaller. But the collaterals do not converge. Table 7 exhibits this phenomenon.

The relationship between the subspace dimension p and the actual number of targets e can be subtle. In a typical scenario, $p > e$ and the collaterals will also converge, except at a slower speed. But in the case when the collaterals do not converge, one might think that there is no fundamental harm in carrying them along except for a moderate increase of computational cost. Theorem 5.2 suggests some potential prob-

TABLE 7

Nonconvergence of collaterals. There are five targets, and subspace dimension p is set to 9. The ratios $|\gamma_{p+1}/\gamma_j| \approx 1$ for $j = 6, 7, 8, 9$ and thus the collateral eigenvalues do not converge. These iterations would have been successful even if p was set to be just 5.

j	$\log_2 \left \frac{\gamma_{10}}{\gamma_j} \right $	Convergence of eigenvalues $\log_2 \left(\lambda_j - \bar{\lambda}_j / \ M\ \right)$ at iteration k					
		$k = 1$	$k = 2$	$k = 3$	$k = 4$	$k = 5$	$k = 6$
1	-9	-38.77	-56.77	-62.87	-63.00	-64.45	-66.45
2	-9	-35.38	-53.39	-61.17	-62.87	-62.65	-62.55
3	-9	-37.50	-55.51	-62.41	-62.37	-63.45	-61.81
4	-9	-36.77	-54.78	-65.55	-65.45	-63.13	-63.00
5	-9	-43.19	-61.21	-63.17	-62.21	-62.13	-64.87
above are e target eigenvalues; below are "collaterals"							
6	-0.0023	-33.53	-35.55	-35.56	-35.56	-35.56	-35.56
7	-0.0017	-32.36	-37.61	-37.62	-37.62	-37.63	-37.63
8	-0.0012	-31.26	-36.75	-36.77	-36.77	-36.77	-36.77
9	-0.0006	-30.29	-35.07	-35.07	-35.07	-35.07	-35.07

lems. Consider the previous example where the nine-dimensional subspaces capture the e target eigenvectors well, but not much of anything else. The reduced systems carry with them two subsystems. One is approximately Λ_e , and the other of the form $H^* \Lambda_{e'} H$ (in the notation of our theorems). If one is unlucky to have the eigenvalues of the second subsystem closely approximating some of the targets, convergence speed of target eigenvalues may be reduced to improvement of $|\gamma_{p+1}/\gamma_e|$ per step, as opposed to $|\gamma_{p+1}/\gamma_e|^2$. More importantly, some of the eigenvectors may actually be wrong! The residual may not converge to zero. We illustrate this phenomenon in the next example. For simplicity, we use a real-valued simple eigenvalue problem of dimension 500. We place just one eigenvalue $\lambda = 16$ in the middle of $[\lambda_-, \lambda_+] = [15, 17]$ but place two eigenvalues at $15 - \zeta$ and $17 + \zeta$ so that $\rho(15 - \zeta) = \rho(17 + \zeta) = 2^{-9}$. The remaining 497 eigenvalues are randomly generated except those at least at a distance of 3 away from $[15, 17]$. We set $p = 2$ and thus the target eigenvalue should converge at least by 2^{-9} per iteration, but usually at 2^{-18} per step. We contrivedly start the iterations with two vectors, one close to the target eigenvector, and the other in about the middle of the two eigenvectors associated with $15 - \zeta$ and $17 + \zeta$. That is, the Rayleigh quotient with this vector is exactly 16. Table 8 illustrates the problem with a small gap between Λ_m and $H^* \Lambda_{m'} H$. As exhibited there, one of the two eigenvalues of the reduced system converges to 16, albeit only improving by 2^{-9} per step. Neither residual vector converges in any practical sense.

6.4. Multiple search intervals and splitting of clusters. Given several search intervals, FEAST can compute eigenpairs within a search interval totally independently. A natural use for this property is to split one large interval into several smaller ones, offering parallelism. As in Experiment 4.1 in [15], we apply this approach to the generalized Hermitian eigenvalue problem specified by the matrix pairs `bcsstk11` and `bcsstm11` from Matrix Market.² We set \mathcal{I} to $[0, 3.85 \times 10^7]$ and partition it into K equal-length (sub)intervals, $K = 1, 2, 3, 4, 5, 10$. Table 9 summarizes the result.

In this next example, FEAST computes eigenpairs of two attaching intervals $[1, 2]$ and $[2, 3]$ of a complex Hermitian eigenvalue problem ($B = I$) of dimension 500. A cluster of eigenvalues $2 \pm \ell \times 10^{-10}$, $\ell = 1, 2, \dots, 5$, is placed around 2. In addition,

²<http://math.nist.gov/MatrixMarket>

TABLE 8

$O(\epsilon^k)$ convergence of eigenvalues and nonconvergence of residual. This artificial example is set up so that there is only one eigenvalue, $\lambda = 16$, in the target interval. With $p = 2$ we have the ratio $\gamma_{p+1}/\gamma_1 = 2^{-9}$. In fact, $\gamma_2/\gamma_1 = 2^{-9}$ as well. The collateral space is affecting the overall convergence. Convergence of the eigenvalue falls back to 2^{-9} per iteration, not at the often enjoyed speed of 2^{-18} per iteration. More importantly, the residual vector is not really converging. The $1/\eta$ factor in Theorem 5.2 is realistic. For this example, convergence will be restored to the perfect situation had p been set to 1.

$p = 2, \left \frac{\gamma_2}{\gamma_1} \right = 2^{-9}$ δ_k is	Convergence hampered by spurious eigenvalues							
	Examine $\log_2(\delta_k/\ A\)$ at iterations k							
	$k = 1$	$k = 2$	$k = 3$	$k = 4$	$k = 5$	$k = 6$	$k = 7$	$k = 8$
$\min_{j=1,2} \bar{\lambda}_j - 16 $	-18.45	-27.46	-37.60	-47.42	-46.00	-46.42	-46.00	-46.19
$\min_{j=1,2} \ A\bar{x}_j - \bar{\lambda}_j \bar{x}_j\ $	-6.13	-6.13	-6.20	-12.66	-15.84	-16.13	-15.92	-16.46

TABLE 9

Matrix market test problem using multiple search intervals. Each of the (sub)intervals is computed with $q = 16$. At most three applications of $\rho(M)$ were required for convergence for both eigenvalues and residual vectors to machine precision. We report the mutual B -orthogonality within one subinterval and across all subintervals: $\text{ortho}_k \stackrel{\text{def}}{=} \max_{i,j} |x_i^* B x_j|$ for all distinct computed eigenvectors from the k th subinterval, $k = 1, 2, \dots, K$. The measure $\text{ortho}_{\text{all}}$ is defined similarly, except computed eigenvectors are drawn from all subintervals.

	Number of equal-length partition of $[0, 3.85 \times 10^7]$					
	1	2	3	4	5	10
$\text{ortho}_{\text{all}}$	3.5×10^{-15}	2.7×10^{-14}	2.5×10^{-14}	2.6×10^{-14}	2.8×10^{-13}	3.6×10^{-13}
$\max_k \text{ortho}_k$	3.5×10^{-15}	5.3×10^{-15}	4.4×10^{-15}	5.4×10^{-15}	8.8×10^{-15}	5.5×10^{-15}
$\min_k \text{ortho}_k$	3.5×10^{-15}	2.8×10^{-15}	2.5×10^{-15}	1.6×10^{-15}	1.9×10^{-15}	9.8×10^{-16}

there are five eigenvalues randomly placed in each of the interiors: $[1.2, 1.8]$ and $[2.2, 2.8]$. The remaining 480 eigenvalues are placed randomly outside of $[1, 3]$ separated by a distance of at least 0.5. Although there are ten eigenvalues in each of the two search intervals, any $p \leq 15$ is detected as small by Algorithm FEAST with the Estimate as all of $\hat{B}_{(k)}$'s eigenvalues are large, due to a large $|\gamma_{p+1}|$. Both search intervals are handled with $p = 16$. In each search interval, all of the associated spectrum together with the entire cluster, 15 eigenpairs in total, is obtained accurately in the sense of residuals at the level of machine roundoff by the fourth iteration.

We now number the 20 eigenvalues inside $[1, 3]$ from small to large. Denote the computed eigenpairs on the “left” and “right” intervals $[1, 2]$ and $[2, 3]$ by $(\hat{\mu}_i, \mathbf{u}_i)$, $(\hat{\nu}_j, \mathbf{v}_j)$, $1 \leq i \leq 15$, and $6 \leq j \leq 20$. Indices from 6 to 15 correspond to those of the eigenvalue cluster. Each of the two sets of 15 eigenvectors are mutually orthonormal. Table 10 shows the orthogonality properties across intervals. The natural strategy in handling two intervals sharing a cluster is to adopt the complete set of eigenpairs for the cluster from just one of the two intervals: $\{(\hat{\mu}_i, \mathbf{u}_i) | 1 \leq i \leq 15\} \cup \{(\hat{\nu}_j, \mathbf{v}_j) | 16 \leq j \leq 20\}$ or $\{(\hat{\mu}_i, \mathbf{u}_i) | 1 \leq i \leq 5\} \cup \{(\hat{\nu}_j, \mathbf{v}_j) | 6 \leq j \leq 20\}$.

6.5. Estimation of eigenvalue count. The number of eigenvalues in $[\lambda_-, \lambda_+]$ is valuable information, but guessing what that number is by counting the number of computed eigenvalues of reduced systems that fall inside $[\lambda_-, \lambda_+]$ is an unsound practice. Theorem 5.3 suggests that we can instead count the number of \hat{B} 's eigenvalues $\geq 1/4$. In the following complex GHEP example of dimension 48, we generated eight

TABLE 10

Splitting a cluster into two search intervals. FEAST is applied on two intervals $[1, 2]$ and $[2, 3]$, each having ten eigenvalues, but the middle 10 of these 20 eigenvalues are clustered around 2, five on the left and five to the right. With subspace dimension set to $p = 16$, computation on each search interval produced 15 accurate eigenpairs: the ten eigenpairs belong to its assigned interval and the five clustering ones in its neighbor. We number the computed eigenpairs on $[1, 2]$ as $(\hat{\mu}_i, \mathbf{u}_i)$, $i = 1, 2, \dots, 15$, and those on $[2, 3]$ as $(\hat{\nu}_j, \mathbf{v}_j)$, $j = 6, 7, \dots, 20$. $\hat{\mu}_i = \hat{\nu}_i$ up to machine roundoff for $i = 6, 7, \dots, 15$. This table examines the orthogonality properties of the computed eigenvectors. The first row illustrates the fundamental nature of sensitivity of eigenvectors of clustering eigenvalues. Rows 2 and 3 show that one can adopt the entire cluster computed from either search interval to obtain a complete spectrum for $[1, 2] \cup [2, 3] = [1, 3]$.

		$\max \mathbf{u}_i^* \mathbf{v}_j $
$6 \leq i \leq 10$	$11 \leq j \leq 15$	1.60×10^{-7}
$1 \leq i \leq 5$	$6 \leq j \leq 20$	1.25×10^{-14}
$1 \leq i \leq 15$	$16 \leq j \leq 15$	1.30×10^{-14}

TABLE 11

Eigenvalue count of $\hat{B}_{(k)}$ to estimate e . In this example, there are exactly $e = 8$ eigenvalues in $[\lambda_-, \lambda_+] = [15, 17]$, $p = 12$. The computed eigenvalues of reduced problem may have more than 8 falling inside $[\lambda_-, \lambda_+]$. But the eigenvalue count of $\hat{B}_{(k)}$ estimates e correctly from iteration 2 onwards.

j	$p = 12$ eigenvalues, μ_j , of $\hat{B}_{(k)}$ at iteration k			
	$k = 2$	$k = 3$	$k = 4$	$k = 5$
1	1.031865	1.042407	1.042588	1.042589
2	1.021825	1.037967	1.041980	1.042530
3	0.999644	1.000591	1.000626	1.000662
4	0.998992	0.999999	1.000000	1.000000
5	0.998206	0.999997	1.000000	1.000000
6	0.996776	0.999936	0.999999	1.000000
7	0.929957	0.999593	0.999857	0.999909
8	0.872044	0.989169	0.998930	0.999845
9	0.201241	0.210605	0.211077	0.211304
10	0.137805	0.146882	0.150190	0.153307
11	0.086650	0.095591	0.098854	0.104075
12	0.050975	0.078311	0.084910	0.088754
$\#\mu_j \geq 1/4$	8	8	8	8
$\#\hat{\lambda}_j \in [\lambda_-, \lambda_+]$	10	9	9	9

eigenvalues inside $[\lambda_-, \lambda_+] = [15, 17]$. We place on each side of $[\lambda_-, \lambda_+]$ 20 random eigenvalues of similar distribution to increase the chance of “spurious” eigenvalues. We set p to 12. Table 11 shows that the distribution of \hat{B} ’s eigenvalues is a much more robust indication of e than that of computed eigenvalues of reduced systems.

Along the same lines, the next example in Table 12 shows that we can get an early indication that p is set too small by the eigenvalues of $\hat{B}_{(k)}$. The example’s setting is similar to the previous one, except p is set to 6, which is two less than the number of eigenvalues inside $[\lambda_-, \lambda_+] = [15, 17]$. The actual computed eigenvalues do not converge, which was to be expected.

7. Conclusions. We have shown that quadrature-based approximate spectral projectors are superb tools to be used with the standard subspace iteration method. This combination is the essence of the recently proposed FEAST algorithm and software [21, 22]. Our detailed analysis establishes FEAST’s convergence properties and shows how its robustness can be further enhanced as methods for counting target eigenvalues and detecting inappropriate subspace dimension are identified. Eigenproblems of large-and-sparse systems fit FEAST naturally as it can tolerate less-accurate solutions of linear systems, allowing the use of iterative linear solvers (see Example 3 in [21]).

TABLE 12

Eigenvalue count of $\widehat{B}_{(k)}$ to judge p . In this example, there are $e = 8$ eigenvalues in $[\lambda_-, \lambda_+] = [15, 17]$. But p is set too small at $p = 6$. Computed eigenvalues will not converge in general. This table illustrates that a too-small p can be detected by examining $\widehat{B}_{(k)}$'s eigenvalues as early as the second iteration. The symptom is that none of $\widehat{B}_{(k)}$'s eigenvalues are less than $1/4$.

j	Computed eigenvalues $\tilde{\lambda}_j$ of reduced system at iteration k				Eigenvalues μ_j of $\widehat{B}_{(k)}$, as a monitor, at iteration k			
	$k = 2$	$k = 3$	$k = 4$	$k = 5$	$k = 2$	$k = 3$	$k = 4$	$k = 5$
1	15.30888	15.30960	15.30709	15.30358	1.03473	1.03600	1.03768	1.03997
2	15.53633	15.54323	15.54300	15.54067	1.01624	1.01788	1.02042	1.02356
3	16.18678	16.21928	16.22838	16.23129	1.00012	1.00016	1.00016	1.00016
4	16.54569	16.58401	16.58713	16.58817	0.99987	1.00002	1.00002	1.00002
5	16.59844	16.63769	16.66165	16.66953	0.99871	0.99984	0.99984	0.99985
6	16.81077	16.83859	16.85640	16.86408	0.74160	0.89480	0.96709	0.99060

Extension of the present work to non-Hermitian problems is a natural next step. Consider for now a simple non-Hermitian eigenvalue problem for a diagonalizable matrix A with an eigendecomposition $A = X \Lambda Y^*$, $XY^* = I$, where Λ is a diagonal matrix and X is a set of right eigenvectors. (Y is a set of left eigenvectors.) Hermitian FEAST is shown here to be subspace iteration with a special accelerator. Subspace iteration, however, is applicable to non-Hermitian problems, either focusing on the right (or left) eigenspace as in [30] or on both eigenspaces (see [4] or [34, page 609]). Furthermore, our approximate spectral projector accelerator is applicable to non-Hermitian matrices as well: Suppose \mathcal{C} is a simple region (e.g., an ellipse) containing a spectrum of interest. Let $\rho(\mu)$ be of the form $\sum_{k=1}^q \alpha_k / (\beta_k - \mu)$, where none of the β_k 's are in A 's spectrum. Then $\rho(A) = X \rho(\Lambda) Y^*$. Provided $|\rho(\lambda)| \approx 1$ for $\lambda \in \text{eig}(A) \cap \mathcal{C}$ and $|\rho(\mu)| \ll 1$ for $\lambda \in \text{eig}(A) \setminus \mathcal{C}$, $\rho(A)$ approximates the (right) spectral projector $X_{\mathcal{C}} Y_{\mathcal{C}}^*$. ($\rho^*(A)$ approximates the left spectral projector $Y_{\mathcal{C}} X_{\mathcal{C}}^*$.) The function $\rho(\mu)$ can be constructed by quadrature rules applied to the Cauchy integral corresponding to \mathcal{C} . For example, define the parametrization for ellipses (similar to (3.2)):

$$\phi_a(t) = \cos\left(\frac{\pi}{2}(1+t)\right) + ia \sin\left(\frac{\pi}{2}(1+t)\right), \quad -1 \leq t \leq 3,$$

for a parameter a , $0 < a < \infty$. A parameter $a < 1$ corresponds to a flat ellipse, and $a > 1$, tall. One can construct a rational function $\rho(\mu)$ by applying a quadrature rule to $\pi(\mu)$ in (3.3), with $\phi_a(t)$ in place of $\phi(t)$. Because A 's spectrum can be complex, we need to study $\rho(\mu)$'s behavior for complex μ . Figure 4 illustrates that indeed the quadrature approach is effective. While more rigorous analysis is needed, the above discussions, supported by positive early experimental results in [16], make the idea of a non-Hermitian FEAST credible.

On a different note, we have used Gauss–Legendre quadrature as our numerical integrator of choice for $\rho(\lambda)$'s accurate approximation to the characteristic function $\pi(\lambda)$ on $[\lambda_-, \lambda_+]$ (see (3.1)). Nevertheless, accurate approximation of $\pi(\lambda)$ is by no means the only relevant property of an integrator suitable for FEAST. Investigation of other quadrature rules is worthwhile. One observation is that $|\rho(\lambda)|$ need not approximate 1 very well on a large portion of $[\lambda_-, \lambda_+]$ or decay to zero outside of $[\lambda_-, \lambda_+]$ —remarkably, both phenomena Gauss–Legendre possesses. It suffices to have, for example, $\rho(\lambda)$ fluctuate as long as $1^+ \geq \rho(\lambda) \geq \eta \gg 0$ on $[\lambda_-, \lambda_+]$ while keeping $|\rho(\lambda)|$ uniformly small outside $[\lambda_- - \delta, \lambda_+ + \delta]$ for some small $\delta > 0$. Another observation is that it is valuable to have a quadrature rule that provides increasing accuracy by progressively adding more nodes (while maintaining those existing). This

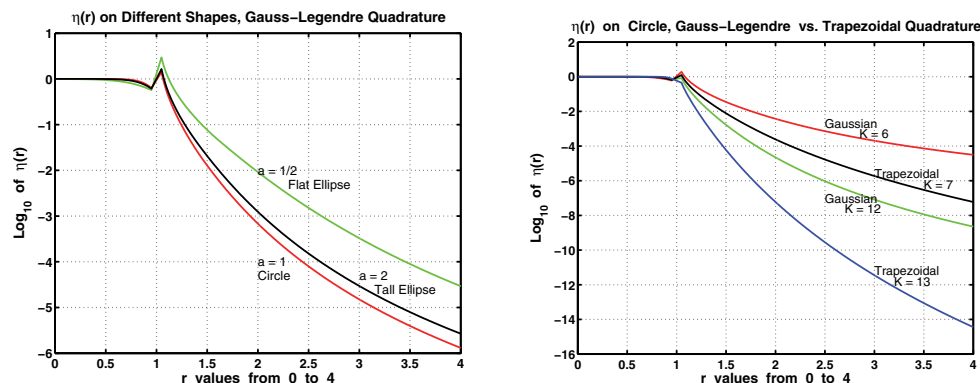


FIG. 4. Let $\mu(r, t) = r[\cos(\frac{\pi}{2}(1+t)) + ia \sin(\frac{\pi}{2}(1+t))]$ for some fixed $a > 0$. Define $\eta(r)$ to be $\min_t |\rho(\mu(r, t))|$ for $0 \leq r \leq 1 - 0.01$, and $\max_t |\rho(\mu(r, t))|$ for $r \geq 1 + 0.01$. The function $\eta(r)$ serves as an indicator of ρ 's behavior as an approximate spectral projector. The plot on the left shows $\rho(\mu)$'s behavior on the complex plane via $\eta(r)$ for Gauss-Legendre $q = 8$ on different elliptical shapes. The plot on the right shows $\rho(\mu)$'s behavior on a circular search region for Gauss-Legendre and trapezoidal quadratures of several different degrees.

would require us to find an alternative to Gauss-Legendre. In short, opportunities for further work are ample.

Acknowledgments. We acknowledge the many fruitful discussions with Prof. Ahmed Sameh and Dr. Faisal Saied of Purdue University, as well as Dr. Victor Kostin and Dr. Sergey Kuznetsov of Intel Corporation. In addition, Sergey Kuznetsov's rigorous testing of multiple versions of the FEAST software was invaluable.

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