

## ON LOWER BOUNDS OF EIGENVALUES FOR SELF ADJOINT OPERATORS

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### 1. Introduction

For the eigenvalue problem of  $Au = \lambda u$  where  $A$  is considered as a semi-bounded self-adjoint operator on a Hilbert space, we are used to apply two complementary methods finding upper bounds and lower bounds to the eigenvalues. The most popular method for finding upper bounds may be the Rayleigh–Ritz method which was developed in the 19th century while a method for computing lower bounds may be the method of intermediate eigenvalue problems which has been developed since 1950's. In the method of intermediate eigenvalue problems (IEP), we consider the original operator eigenvalue problem as a perturbation of a simpler, resolvable, self-adjoint eigenvalue problem, called a base problem, that gives rough lower bounds. The intermediate eigenvalue estimates are obtained by computing the spectrum of the base operator summed with a positive semi-definite finite rank operator. But intermediate problem methods have some defects. They require practically not only explicit knowledge of reducing spaces and spectrum of the base operator but also special choices for the range space of the approximating finite rank operators. This makes the resulting problem have dense matrices so that they may be difficult to handle practically on available computational resources. These practical obstructions come from the explicit involvement of the base problem eigenfunctions which are typically supported throughout the problem domain.

The so-called eigenvector free method (EVF) which was developed recently by Beattie and Goerisch [5] may overcome such problems since it does not need information of eigenfunctions of the base problem and permits the use of finite-element trial functions so that it yields final

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computational matrices which are sparse and well-structured. Bounds are obtained from generalized symmetric matrix eigenvalue problems. Highly accurate bounds require large order of matrix problem which may not be practical to use the  $QZ$  method [10] which is not able to use any existing sparsity in the original coefficient matrices. For large order problems, the necessity of retaining the sense of these derived bounds in the face of finite-precision arithmetic leads to the consideration of iterative algorithms having a variational component. Such a component provides intermediate results at every step that may be used to deduce rigorous bounds, even the method terminates prematurely.

In this paper we find a relationship of eigenpairs between an IEP method and the EVF method. We also show how to get lower bounds with an iteration method to use the sparsity of the matrices. Finally we show how to use a Ritz value to make the number of iterations so small. In Section 2 we review the EVF method of Beattie and Goerisch and give a relationship of eigenpairs between EVF and IEP methods. Section 3 deals with how to take advantage of the sparsity of large-order matrix eigenvalue problems as well as how to choose shifts to make the number of iterations small. With these shifts we compute in Section 4 vibrational frequencies of a clamped plate on rectangular domains.

## 2. On the eigenpair of EVF and IEP methods

In this section we describe the EVF method briefly and show a relationship of eigenpairs between the EVF method and an IEP method. For more details on the EVF method, one should refer to [5] and for the IEP, refer to [3,15].

Let  $\mathcal{H}$  be a separable Hilbert space with a norm  $\|\cdot\|$  and an inner product  $\langle \cdot, \cdot \rangle$ . Let  $A$  be a self adjoint operator with domain dense in  $\mathcal{H}$  which is bounded below, and let the spectrum consists of a finite or infinite number of isolated eigenvalues

$$\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_\infty$$

on its lower part, each having finite multiplicity. Here  $\lambda_\infty$  means the least limit point of the spectrum of  $A$ . We denote  $a(\cdot)$  by the quadratic form which is the closure of  $\langle A\cdot, \cdot \rangle$ . We assume that a self adjoint

operator  $A_0$  is taken to be bounded below and  $A_0 \leq A$ , and that the isolated eigenvalues of  $A_0$

$$\lambda_1^0 \leq \lambda_2^0 \leq \dots \leq \lambda_\infty^0$$

are known. We assume that the quadratic form  $a(u)$  is decomposed as

$$a(u) = a_0(u) + \|Tu\|_*^2$$

where  $T$  is a closed operator on  $\mathcal{H}$  to another Hilbert space  $\mathcal{H}_*$ .

Let  $T^*$  be the adjoint operator of  $T$ . We take a sequence of finite dimensional spaces  $\{\mathcal{P}_k\}$  such that

$$\mathcal{P}_1 \subset \mathcal{P}_2 \subset \dots \subset \mathcal{P}_k \subset \mathcal{P}_{k+1} \subset \dots \subset \text{Dom}(T^*) \subset \mathcal{H}_*$$

and let  $P_k : \mathcal{H}_* \rightarrow \mathcal{P}_k$  be the projection that is orthogonal with respect to the inner product  $\langle \cdot, \cdot \rangle_*$ . We construct the intermediate quadratic forms  $a_k(u)$  as

$$a_k(u) = a_0(u) + \|P_k T u\|_*^2$$

for all  $u \in \text{Dom}(a_k) = \text{Dom}(a_0) \cap \text{Dom}(T)$ , which may be associated with a self-adjoint operator given by

$$A_k = A_0 + T^* P_k T$$

with  $\text{Dom}(A_k) = \text{Dom}(A_0)$ .

For any constant  $\delta$ , the operator  $A_k$  may be rewritten by

$$A_k = (A_0 - \delta^2) + (T^* P_k T + \delta^2).$$

Let  $B_k = T^* P_k T + \delta^2$  for each  $k$ . The operator  $B_k$  produces a new inner product  $\langle B_k \cdot, \cdot \rangle$  on the Hilbert space  $\mathcal{H}$ . Let a sequence of finite dimensional subspaces  $\{\hat{\mathcal{P}}_k\}$  be given such that

$$\hat{\mathcal{P}}_1 \subset \hat{\mathcal{P}}_2 \subset \dots \subset \hat{\mathcal{P}}_n \subset \hat{\mathcal{P}}_{n+1} \subset \dots \subset \mathcal{H}$$

and let  $\hat{P}_n : \mathcal{H} \rightarrow \hat{\mathcal{P}}_n$  be the projection that is orthogonal with respect to this inner product  $\langle B_k \cdot, \cdot \rangle$ . We form the intermediate operators as

$$A_{k,n} = (A_0 - \delta^2) + B_k \hat{P}_n.$$

The associated  $n \times n$  Weinstein and Aronszajn(W-A) matrix of the operator  $A_{k,n}$  is given by

$$(2.1) \quad W_{k,n}(\lambda) = [\langle \hat{p}_i + R_{\lambda+\delta^2}^0 B_k \hat{p}_i, B_k \hat{p}_j \rangle]$$

for  $i, j = 1, \dots, n$ , where  $R_\mu^0$  is the resolvent operator,  $(A_0 - \mu)^{-1}$ , of  $A_0$  at  $\mu$ . If we let  $\mu = \lambda + \delta^2$  and introduce the change of variable  $q_i = R_\mu^0 B_k \hat{p}_i$  into the W-A matrix (2.1), we get

$$W_{k,n}(\lambda) = [\langle B_k^{-1}(A_0 - \mu)q_i, (A_0 - \mu)q_j \rangle + \langle q_i, (A_0 - \mu)q_j \rangle]$$

which is more simplified with a formula for  $B_k^{-1}$ (see [1,2]) to get

$$W_{k,n}(\lambda) = [\langle q_i, (A_0 - \mu)q_j \rangle + \frac{1}{\mu - \lambda} \{ \langle (A_0 - \mu)q_i, (A_0 - \mu)q_j \rangle - \sum_{l,m=1}^k \langle (A_0 - \mu)q_i, T^* p_l \rangle c_{lm} \langle T^* p_m, (A_0 - \mu)q_j \rangle \}].$$

If we define the matrices as

$$F_1 = [\langle q_i, (A_0 - \mu)q_j \rangle], \quad F_2 = [\langle p_i, p_j \rangle_*], \quad H = [\langle (A_0 - \mu)q_i, T^* p_j \rangle] \\ G_1 = [\langle (A_0 - \mu)q_i, (A_0 - \mu)q_j \rangle], \quad G_2 = [\langle T^* p_i, T^* p_j \rangle],$$

then the W-A matrix is compactly expressed as

$$(2.2) \quad W_{k,n}(\lambda) = F_1 + \frac{1}{\mu - \lambda} \{ G_1 - H[(\mu - \lambda)F_2 + G_2]^{-1} H^* \}.$$

Based on this W-A matrix, Beattie and Goerisch introduced the EVF method. For more general case, refer to [5].

**THEOREM 2.1.** (Beattie and Goerisch) *Let  $\mu$  and  $r$  be chosen so that  $\lambda_{r-1}^0 < \mu \leq \lambda_r^0$ . Suppose that  $\{p_i\}_{i=1}^k \subset \text{Dom}(T^*)$  and  $\{q_i\}_{i=1}^n \subset \text{Dom}(A_0)$  such that  $\{(A_0 - \mu)q_i\}_{i=1}^n$  and  $\{T^* p_i\}_{i=1}^k$  are jointly linearly independent. If the generalized matrix eigenvalue problem*

$$(2.3) \quad \begin{bmatrix} F_1 & 0 \\ 0 & F_2 \end{bmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \xi \begin{bmatrix} G_1 & H \\ H^* & G_2 \end{bmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

has discrete finite eigenvalues ordered as

$$\xi_1 \leq \xi_2 \leq \dots \leq \xi_l < 0 \leq \xi_{l+1} \leq \dots,$$

then for each eigenvalue  $\xi_p$  with  $p \leq l$  we have a corresponding lower bound to an eigenvalue of  $A$ ;

$$\mu + \frac{1}{\xi_p} \leq \lambda_{r-p}.$$

If  $\{q_i\}_{i=1}^n$  and  $\{p_j\}_{j=1}^k$  are chosen to have local support as with finite-element trial functions, we note then that the resulting matrices will be sparse and the matrix eigenvalue problem may be efficiently handled using sparse techniques, even for quite large values of  $n$  and  $k$ .

We next consider a relation between eigenpairs of the matrix pencil (2.3) and those of intermediate operators  $A_{k,n}$ . Let  $u$  be an eigenfunction of  $A_{k,n}$  corresponding to an eigenvalue  $\lambda$  which is not an eigenvalue of  $A_0 - \delta^2$ . Then  $\lambda$  satisfies the determinantal equation of  $W$ - $A$  matrix (2.1) and  $u = \sum_{j=1}^n \alpha_j R_{\lambda+\delta^2}^0 B_k \hat{p}_j$  with  $\alpha = (\alpha_1, \dots, \alpha_n)^T \in \ker W_{k,n}(\lambda)$ . Let  $\mu = \lambda + \delta^2$ . Then there is a positive integer  $r$  such that  $\lambda_{r-1}^0 < \mu \leq \lambda_r^0$ . If we let  $q_j = R_\mu^0 B_k \hat{p}_j$ , we have

$$F_1 \alpha = \xi \{G_1 - H[-\frac{1}{\xi} F_2 + G_2]^{-1} H^* \} \alpha$$

with  $\xi = \frac{1}{\lambda - \mu} = -\frac{1}{\delta^2}$  and  $u = \sum_{j=1}^n \alpha_j q_j$ . If we define

$$(2.5) \quad \beta = \xi(F_2 - \xi G_2)^{-1} H^* \alpha,$$

the vector  $\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$  is an eigenvector of (2.3) corresponding to an eigenvalue  $\xi$ . Conversely, let  $\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$  be an eigenvector of (2.3) corresponding to an eigenvalue  $\xi$  for fixed  $\mu$ . Then

$$F_1 \alpha = \xi \{G_1 - H[-\frac{1}{\xi} F_2 + G_2]^{-1} H^* \} \alpha.$$

Therefore  $u = \sum_{j=1}^n \alpha_j q_j$  is an eigenvector of  $A_{k,n}$  with  $\delta^2 = -\frac{1}{\xi}$  corresponding to an eigenvalue  $\lambda = \mu + \frac{1}{\xi}$ , which leads to the following.

**THEOREM 2.2.** *If  $\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$  is an eigenvector of the matrix pencil (2.3) with a corresponding eigenvalue  $\xi$ , then  $\sum_{j=1}^n \alpha_j q_j$  is an eigenvector of intermediate operator  $A_{k,n}$  with  $\delta^2 = -\frac{1}{\xi}$  which corresponds to an eigenvalue  $\mu + \frac{1}{\xi}$ . Conversely if  $u$  is an eigenfunction of  $A_{k,n}$  corresponding to  $\lambda$  for fixed  $\delta^2$ , then for  $\mu = \lambda + \delta^2$ ,  $-\frac{1}{\delta^2}$  is an eigenvalue of (2.3) corresponding to the eigenvector  $\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$  with  $\alpha \in \ker W_{k,n}(\lambda)$  and  $\beta$  in (2.5).*

For obtaining a close relationship of eigenvalues between EVF and IEP, we define for  $\theta > 0$  by  $A_{k,n}^\theta = A_0 - \theta I + (T^* P_k T + \theta I) P_n^{(k,\theta)}$ . Note that  $W_{k,n}^\theta(\lambda) = M_{k,n}(\xi) / (F_2 - \xi G_2)$  with  $\xi = -\frac{1}{\theta}$  and  $\theta = \mu - \lambda$  which is the Schur complement of  $M_{k,n}(\xi)$  with respect to  $F_2 - \xi G_2$  (see [7]). Here

$$M_{k,n}(\xi) = \begin{bmatrix} F_1 & 0 \\ 0 & F_2 \end{bmatrix} - \xi \begin{bmatrix} G_1 & H \\ H^* & G_2 \end{bmatrix}$$

Since  $F_2$  (or  $G_2$ ) is positive definite, for any  $\xi < 0$  the determinant of  $F_2 - \xi G_2$ ,  $|F_2 - \xi G_2|$ , does not vanish. Thus  $|W_{k,n}^\theta(\lambda)| \cdot |F_2 - \xi G_2| = |M_{k,n}(\xi)|$  (see [7]). Let  $\lambda^{(k,n,\theta)}$  be an eigenvalue of  $A_{k,n}^\theta$  for fixed  $\theta$ . For  $\mu = \lambda^{(k,n,\theta)} + \theta$ , we have

$$|W_{k,n}^\theta(\lambda^{(k,n,\theta)})| \cdot |F_2 + \frac{1}{\theta} G_2| = |M_{k,n}(-\frac{1}{\theta})|.$$

Since  $|W_{k,n}^\theta(\lambda^{(k,n,\theta)})|$  equals zero, we have  $-\frac{1}{\theta}$  as an eigenvalue of  $M_{k,n}$  with  $\mu = \lambda^{(k,n,\theta)} + \theta$ . Conversely, for fixed  $\mu$ , let  $\xi < 0$  be an eigenvalue of  $M_{k,n}$ . i.e.,  $|M_{k,n}(\xi)| = 0$ . Since  $|F_2 - \xi G_2| \neq 0$ , we have  $|W_{k,n}^\theta(\mu + \frac{1}{\xi})| = 0$  with  $\theta = -\frac{1}{\xi}$ . It follows that  $\mu + \frac{1}{\xi}$  is an eigenvalue of  $A_{k,n}^\theta$  with  $\theta = -\frac{1}{\xi}$ .

**THEOREM 2.3.** For any  $p$  with  $1 \leq p \leq l$ ,  $\mu + \frac{1}{\xi_p}$  is equal to the  $(r - p)$ th eigenvalue,  $\lambda_{r-p}^{(k,n,-\frac{1}{\xi_p})}$ , of  $A_{k,n}^{-\frac{1}{\xi_p}}$ .

*Proof.* Let  $N_{k,n}^\theta(\lambda)$  be the number of eigenvalues of  $A_{k,n}^\theta$  strictly less than  $\lambda$ . For  $\theta = -\frac{1}{\xi_p}$ ,  $N_{k,n}^\theta(\mu + \frac{1}{\xi_p}) = r - p - 1$  (See [5]). Thus we have

$$\lambda_{r-p-1}^{(k,n,-\frac{1}{\xi_p})} < \mu + \frac{1}{\xi_p} \leq \lambda_{r-p}^{(k,n,-\frac{1}{\xi_p})}.$$

By the argument above,  $\mu + \frac{1}{\xi_p}$  is an eigenvalue of  $A_{k,n}^{-\frac{1}{\xi_p}}$  and thus  $\mu + \frac{1}{\xi_p}$  should be equal to  $\lambda_{r-p}^{(k,n,-\frac{1}{\xi_p})}$ .

### 3. Numerical realization of eigenvalue bounds

We deal with large order matrix eigenvalue problem which comes from the EVF method. For this purpose, we consider the generalized matrix eigenvalue problem

$$(3.1) \quad \mathcal{A}x = \xi \mathcal{B}x$$

where  $\mathcal{A}$  is a symmetric positive definite matrix and  $\mathcal{B}$  is a symmetric positive semi-definite matrix. Many different approaches exist for computing selected eigenvalues of (3.1) when  $\mathcal{A}$  and  $\mathcal{B}$  are very large and very sparse. The simplest of these is a subspace iteration. But we are interested in a few eigenvalues. Hence the spectral transformation Lanczos method (STLM) may be useful. If one is willing to live with the expense of a factorization of  $\mathcal{A} - \sigma \mathcal{B}$ , STLM is often substantially more effective than subspace iteration. Moreover, if  $\mathcal{B}$  is singular, STLM does not suffer the same degradation of the accuracy [11]. With a shift  $\sigma$ , equation (3.1) is transformed to

$$(3.2) \quad (\mathcal{A} - \sigma \mathcal{B})^{-1} \mathcal{B}x = \frac{1}{\xi - \sigma} x.$$

For convenience, let  $\mathcal{M} = (\mathcal{A} - \sigma\mathcal{B})^{-1}\mathcal{B}$ . All eigenvectors of (3.1) corresponding to finite eigenvalues are also eigenvectors of  $\mathcal{M}$ , and they lie in the range of  $\mathcal{M}$ . The semi-inner product induced by  $\mathcal{B}$  is a true inner product on the range of  $\mathcal{M}$ , and also the eigenvalue problem (3.2) is self-adjoint with respect to this inner product even though the problem is not symmetric [11]. STLM requires calculating the action of  $\mathcal{M}$  on a vector of the range of  $\mathcal{M}$  at each iteration step. It constructs a symmetric tridiagonal matrix,  $T_j \in \mathbb{R}^{j \times j}$ , in the course of  $j$  iteration steps, whose eigenvalues approximate those of (3.2). A set of Lanczos vectors  $\{q_i\}_{i=1}^j$  that form a  $\mathcal{B}$ -orthogonal basis for the order  $j$  Krylov subspace is generated by  $\mathcal{M}$  and  $q_1$ . In floating point arithmetic,  $\mathcal{B}$ -orthogonality is volatile and expensive to maintain, but so long as the  $\{q_i\}_{i=1}^j$  are kept robustly independent ( $\mathcal{B}$ -"semiorthogonal"), one can guarantee up to terms on the order of the machine precision that  $T_j$  is the Rayleigh-Ritz restriction of (3.2) to  $\text{span}(\{q_i\}_{i=1}^j)$  with respect to the  $\mathcal{B}$ -inner product [13]. The eigenvalues of  $T_j$  will be associated with **upper** bounds to corresponding eigenvalues of (3.2) and thus it will be associated with **lower** bounds to corresponding eigenvalues of (3.1).

On the other hand, the eigenvalues of the given operator from the EVF method are associated with lower bounds according to

$$\mu + \frac{1}{\xi_p} \leq \lambda_{r-p}$$

for each  $p = 1, 2, \dots, r-1$ . If  $\hat{\xi}_p \geq \xi_p$  is an estimate of  $\xi_p$ , then  $\mu + (1/\hat{\xi}_p) \leq \mu + (1/\xi_p) \leq \lambda_{r-p}$ . Hence we must seek **upper** bounds to the negative eigenvalues of (2.3) or (3.1) so as to maintain consistent lower bounds to  $\{\lambda_i\}_1^{r-1}$ . If  $m$  is to be taken practically such that  $\Lambda_m < \mu \leq \Lambda_{m+1}$ , where  $\Lambda_m$  denotes the  $m$ -th Ritz bound corresponding to the eigenvalue  $\lambda_m$ , then it makes sense to find lower bounds only to  $\{\lambda_i\}_1^m$  because  $\mu$  may be already a lower bound to the other ones  $\{\lambda_i\}_{m+1}^{r-1}$  and thus  $\mu + \frac{1}{\xi_p}$ , for  $p = 1, \dots, r-m-1$ , may be worse than  $\mu$  to them. Thus we need at most  $m$  biggest negative eigenvalues of  $\{\xi_i\}$  instead of the entire set of negative eigenvalues.

Let  $\mathcal{A} = \begin{bmatrix} F_1 & 0 \\ 0 & F_2 \end{bmatrix}$  and  $\mathcal{B} = \begin{bmatrix} G_1 & H \\ H^* & G_2 \end{bmatrix}$ . Now we consider how to



select the shift  $\sigma$  for the equation (3.1). It is desirable to choose a zero shift in order to preserve the sparsity of  $\mathcal{A}$ . However, small magnitude eigenvalues may need many iterations to get a reasonable accuracy. In our model of the clamped plate problem the negative eigenvalues of  $(\mathcal{A}, \mathcal{B})$  have very small magnitudes compared to the extreme positive eigenvalues. Moreover, the number of Lanczos steps required exceeds half of the size of its computational matrix to get a reasonable accuracy. In order to overcome such trouble, it may be possible to take a shift so that the wanted eigenvalue of  $\mathcal{M}$  has the biggest magnitude. For this purpose, let  $m$  be such that  $\Lambda_m < \mu$  and let  $p = r - m$ . If we take  $\sigma = (\Lambda_m - \mu)^{-1}$ , it could be then  $\xi_{r-m-1} < \sigma < \xi_{r-m}$ . Without loss of generality we may assume that  $\sigma$  is closer to  $\xi_{r-m}$  than to  $\xi_{r-m-1}$  since  $\Lambda_m$  can be taken to be closer to  $\lambda_m$  than to  $\lambda_{m+1}$ .

If  $\nu_i$ 's are the ordered eigenvalues of  $(\mathcal{A} - \sigma\mathcal{B})^{-1}\mathcal{B}$ , then we have

$$\xi_{r-m} = \frac{1}{\nu_S} + \sigma, \dots, \xi_{r-1} = \frac{1}{\nu_{S-m+1}} + \sigma,$$

where  $S$  is the rank of  $\mathcal{B}$ . We note that the eigenvalue  $\nu_S$  has the biggest magnitude. Since we only need few extreme eigenvalues,  $\nu_S, \dots, \nu_{S-m+1}$ , of  $(\mathcal{A} - \sigma\mathcal{B})^{-1}\mathcal{B}$ , the Lanczos method is expected to be quite efficient. Moreover, if  $\mathcal{A}$  and  $\mathcal{B}$  are large and sparse, we can efficiently reduce the storage for  $\mathcal{A}$  and  $\mathcal{B}$  as storing only their nonzero entries because the STLM requires calculating the action of  $(\mathcal{A} - \sigma\mathcal{B})^{-1}\mathcal{B}$  on a vector at each iteration step, even if it needs additional storage for factorization of  $(\mathcal{A} - \mathcal{B})$ .

Since we seek upper bounds to the negative eigenvalues of (2.3) or (3.1), we have to find lower bounds to the corresponding eigenvalues of  $(\mathcal{A} - \sigma\mathcal{B})^{-1}\mathcal{B}$ . It is appropriate to comment here that the modifications to Rutishauser's subspace iteration *ritzit* ([12]) that extend its applicability to (3.1) are straight-forward, but the resulting eigenvalue estimates are **lower** bounds to  $\xi_i$  of (3.1). Hence it is impossible to directly deduce upper bounds to  $\lambda_i$ . Remarkably, it can be recovered with a rank-one modification of  $T_j$  and so regain the sense of derived bounds for  $\lambda_j$ . We give a brief description. For more detail, one may refer to [11]. Let  $T_j = Q_j^* \mathcal{B} (\mathcal{A} - \sigma\mathcal{B})^{-1} \mathcal{B} Q_j$  be the tridiagonal matrix in STLM and define  $W_j = Q_j^* (\mathcal{A} - \sigma\mathcal{B}) Q_j$ , where  $Q_j$  is a matrix whose columns are Lanczos vectors. Then the eigenvalues of  $W_j$  are the Ritz

value approximations to  $\xi_i - \sigma$  and thus the eigenvalues of  $W_j^{-1}$  are lower bounds to  $\nu_i$  which we want. Moreover, the matrix  $W_j^{-1}$  differs from  $T_j$  only in the last diagonal entry. Hence we easily modify the Lanczos algorithm for our goal. The following is a modified algorithm with full reorthogonalization.

Set  $q_0 = 0$  and take  $r_1 \in \text{ran}(\mathcal{M})$  and let  $\beta_1 := \|r_1\|$ .

For  $j = 1, \dots, \text{maxit}$ , do

$$q_j \leftarrow \frac{r_j}{\beta_j} \quad (\text{normalization})$$

$$\alpha_j \leftarrow q_j^t \mathcal{B} \mathcal{M} q_j$$

$$\text{if } j = 1; \quad \omega_1 \leftarrow q_1^t (\mathcal{A} - \sigma \mathcal{B}) q_1 \text{ and } \mu_1 \leftarrow \frac{1}{\omega_1} - \alpha_1$$

$$\text{else; } \quad \mu_j \leftarrow -\alpha_j - \frac{\beta_j^2}{\mu_{j-1}}$$

$$r \leftarrow (\mathcal{M} - \alpha_j) q_j - \beta_j q_{j-1}$$

$$r_{j+1} \leftarrow r - \sum_{i=1}^j q_i (q_i^t \mathcal{B} r) \quad (\text{orthogonalization})$$

$$\beta_{j+1} \leftarrow (r_{j+1}^t \mathcal{B} r_{j+1})^{\frac{1}{2}} \quad (\text{norm of } r_{j+1} \text{ with respect to } \mathcal{B})$$

$$\alpha_{\text{maxit}} \leftarrow \alpha_{\text{maxit}} + \mu_{\text{maxit}}.$$

#### 4. Application to a clamped plate problem

In this section we give rigorous upper and lower bounds to vibrations of uniform clamped plates on a rectangular domain. The estimation of these vibrations has been treated previously in [4,15]. The lower bounds are obtained by the EVF method using bicubic spline functions as trial functions, while the upper bounds are obtained by the finite element method using the same trial functions.

Let  $\Omega$  denote the open rectangle  $(-\frac{a}{2}, \frac{a}{2}) \times (-\frac{b}{2}, \frac{b}{2})$  in  $\mathbb{R}^2$ . Consider the following simple model of vibration of a clamped plate:

$$\Delta^2 u = \lambda u \text{ on } \Omega \quad \text{with} \quad u = \frac{\partial u}{\partial n} = 0 \text{ on } \partial\Omega.$$

That is, the operator  $A$  is defined on a core of  $C_0^\infty(\Omega) \subset L^2(\Omega) = \mathcal{H}$  by

$$Au = \frac{\partial^4 u}{\partial x^4} + \frac{\partial^4 u}{\partial y^4} + 2 \frac{\partial^4 u}{\partial x^2 \partial y^2} \quad \text{with} \quad u = \frac{\partial u}{\partial n} = 0 \text{ on } \partial\Omega.$$

We now define a base operator  $A_0$  on a core of  $C_0^\infty(\Omega) \subset L^2(\Omega)$  by

$$A_0 u = 2 \frac{\partial^4 u}{\partial x^2 \partial y^2} \quad \text{with} \quad u = 0 \text{ on } \partial\Omega$$

and  $T$  on a core of  $C_0^\infty(\Omega) \subset L^2(\Omega)$  into  $L^2(\Omega) \times L^2(\Omega) = \mathcal{H}_*$  by

$$Tu = \left\{ \frac{\partial^2 u}{\partial x^2}, \frac{\partial^2 u}{\partial y^2} \right\} \quad \text{with} \quad u = \frac{\partial u}{\partial n} = 0 \text{ on } \partial\Omega.$$

The adjoint operator  $T^*$  of  $T$  is then obtained on sufficiently smooth functions of  $L^2(\Omega) \times L^2(\Omega)$  by

$$T^*(v, w) = -\left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} \right)$$

with free boundary conditions.

Notice that the region, the differential equation and the boundary conditions, share common properties of symmetry. Thus we can take advantage of this so that we restrict the problem on the space of functions which are even with respect to both x-axes and y-axes. Then we need extra boundary conditions of

$$\frac{\partial u}{\partial n} = 0 \text{ on } \{(0, y), (x, 0) \mid 0 < x < \frac{a}{2} \text{ and } 0 < y < \frac{b}{2}\}.$$

We define  $\Omega = (0, \frac{a}{2}) \times (0, \frac{b}{2})$ ,  $\Gamma_1 = \{(\frac{a}{2}, y), (x, \frac{b}{2}) \mid 0 < x < \frac{a}{2} \text{ and } 0 < y < \frac{b}{2}\}$  and

$$\Gamma_2 = \{(0, y), (x, 0) \mid 0 < x < \frac{a}{2} \text{ and } 0 < y < \frac{b}{2}\}.$$

The boundary conditions for  $A, A_0$  and  $T^*$  restricted to even-even symmetry class are as follows:

- (1) For  $A, u = \frac{\partial u}{\partial n} = 0$  on  $\Gamma_1$  and  $\frac{\partial u}{\partial n} = 0$  on  $\Gamma_2$
- (2) For  $A_0, u = 0$  on  $\Gamma_1$  and  $\frac{\partial u}{\partial n} = 0$  on  $\Gamma_2$
- (3) For  $T^*, \frac{\partial u}{\partial n} = 0$  on  $\Gamma_2$ .

The eigenvalues of  $A_0$  with these boundary conditions are easily found to be

$$\frac{2\pi^4}{a^2b^2}(2i - 1)^2(2j - 1)^2 \text{ for } i, j \geq 1.$$

Now we are in a position to construct approximating vectors for both the EVF and the Rayleigh-Ritz methods. Let  $N \times N$  finite-element mesh be overlaid on  $\Omega$ . Trial functions will be constructed from the associated set of bicubic splines so as to satisfy necessary boundary conditions. Let  $B_i$  be cubic spline functions on  $[0, 1]$  for  $i = -1, \dots, N + 1$ . For approximating vectors within  $Dom(A_0)$ , we define

$$\begin{aligned} \tilde{B}_0 &= B_0, & \tilde{B}_1 &= B_1 + B_{-1} \\ \tilde{B}_j &= B_j, & \text{for } j &= 2, \dots, N - 2 \\ \tilde{B}_{N-1} &= 4B_{N-1} - B_N, & \tilde{B}_N &= 4B_{N+1} - B_N. \end{aligned}$$

Then the approximating vectors are defined as  $q_{ij}(x, y) = \tilde{B}_i(x)\tilde{B}_j(y)$  for  $0 \leq i, j \leq N$  so that the dimension of the finite element space for  $Dom(A_0)$  is  $(N + 1)^2$ . For approximating vectors within  $Dom(T^*)$ , define

$$\begin{aligned} \hat{B}_0 &= B_0, & \hat{B}_1 &= B_1 + B_{-1} \\ \hat{B}_j &= B_j, & \text{for } j &= 2, \dots, N + 1. \end{aligned}$$

Then the approximating vectors are defined as  $\{\hat{B}_i(x)B_j(y), 0\}$  and  $\{0, B_k(x)\hat{B}_l(y)\}$  for  $0 \leq i, l \leq N + 1$  and  $-1 \leq j, k \leq N + 1$  so that

the dimension is  $2(N + 2)(N + 3)$ . Thus we have  $n = (N + 1)^2$  and  $k = 2(N + 2)(N + 3)$  for the EVF method.

For upper bounds, we define

$$\begin{aligned} \bar{B}_0 &= B_0, & \bar{B}_1 &= B_1 + B_{-1} \\ \bar{B}_j &= B_j, & \text{for } j &= 2, \dots, N - 2 \\ \bar{B}_{N-1} &= B_{N-1} - \frac{1}{2}B_N + B_{N+1}. \end{aligned}$$

The approximating vectors for  $Dom(a)$  are defined by  $\phi_{ij}(x, y) = \bar{B}_i(x)\bar{B}_j(y)$  for  $0 \leq i, j \leq N - 1$  so that we have  $n = N^2$  for the Rayleigh–Ritz problem.

For the computation of each entry of the matrices of EVF and Rayleigh–Ritz problem, we need not compute all the integrations that come from the inner products of approximating vectors directly. Instead, we need only find 4 local overlap matrices of dimension  $4 \times 4$  and later compute matrix entries by assembly. For this purpose we denote by  $S_{-1}, S_0, S_1$  and  $S_2$  the cubic spline functions on  $[0, 1]$  with mesh size of 1. Let  $S'_i$  and  $S''_i$  be the first and second derivatives of  $S_i$ . Then we have the following local  $4 \times 4$  matrices:

$\langle S_i, S_j \rangle$			
1/7	129/140	3/7	1/140
129/140	297/35	933/140	3/7
3/7	933/140	297/35	129/140
1/140	3/7	129/140	1/7

$\langle S_i, S''_j \rangle$			
1.2	-2.1	0.6	0.3
9.9	-13.2	-3.3	6.6
6.6	-3.3	-13.2	9.9
0.3	0.6	-2.1	1.2

$\langle S'_i, S'_j \rangle$			
1.8	2.1	-3.6	-0.3
2.1	10.2	-8.7	-3.6
-3.6	-8.7	10.2	2.1
-0.3	-3.6	2.1	1.8

$\langle S''_i, S''_j \rangle$			
12	-18	0	6
-18	36	-18	0
0	-18	36	-18
6	0	-18	12

Let  $B_i$ 's be the cubic spline functions on  $[0, \ell]$  with  $N$  uniform meshes and let  $h = \frac{\ell}{N}$ . Then the global  $N + 3$  by  $N + 3$  matrices  $\{\langle B_i, B_j \rangle\}, \{\langle B''_i, B''_j \rangle\}, \{\langle B_i, B''_j \rangle\}$  and  $\{\langle B'_i, B'_j \rangle\}$  are obtained by assembling the corresponding local matrices and multiplying by  $h, \frac{1}{h^3}, \frac{1}{h}$  and  $\frac{1}{h}$ , respectively. Moreover each entry of the matrices  $\left[\langle \tilde{B}_i, \tilde{B}_j \rangle\right], \left[\langle \bar{B}_i, \bar{B}_j \rangle\right]$  and  $\left[\langle \hat{B}_i, \hat{B}_j \rangle\right]$  with matrices of their derivatives are formed to be a linear combination of each entries of  $\{\langle B_i, B_j \rangle\}$  with matrices of its derivatives. From these, the final matrices  $F_1, F_2, G_1, G_2$ , and  $H$  are built. The  $(i, j)$  entry of each matrix is expressible as the sum of  $4 - |i - j|$  integrals of polynomials of degree 6 or less over some, up to 4, consecutive subintervals  $[x_k, x_{k+1}]$  with  $x_k = \frac{k}{N}$  and  $0 \leq k \leq n - 1$ . These integrals may be computed analytically in principle but this may be highly tedious. Since each integrand is a polynomial of degree no greater than 6, a Gauss quadrature rule with 4-points is adequate to compute exactly each subinterval integration. We note that the inner products of cubic spline functions  $B_i$  and  $B_j$  vanish if the difference between  $i$  and  $j$  is greater than or equal to 4 (i.e.,  $|i - j| \geq 4$ ). The inner product matrices  $F_1, F_2, G_1, G_2$  and  $H$  have a full-band width of 7. Thus the matrix  $\mathcal{A} - \sigma \mathcal{B}$  and  $\mathcal{B}$  have at most  $441N^2 + 196N + 103$  nonzero entries. If we store only the nonzero entries of the matrix, then the size of storage may be reduced from  $O(N^4)$  to  $O(N^2)$  even though additional storage for factorization of  $(\mathcal{A} - \sigma \mathcal{B})$  is needed. In the following table, we show upper and lower bounds for rectangular clamped plate problem. Here the upper bounds come from Rayleigh-Ritz problem of  $N = 35$ .

Table : Vibration of a clamped rectangular plate;  $a = 4$  and  $b = 3$   
(even-even symmetry class)

shift( $\Lambda_m$ )	10.2	79.4	198.0	370.5
N	$\lambda_1$	$\lambda_2$	$\lambda_3$	$\lambda_4$
Base	1.3529040	12.176136	12.176136	33.822601
8	10.1694382	79.3704740	197.847513	370.014443
12	10.1694950	79.3813653	197.897575	370.352315
16	10.1695108	79.3833273	197.906415	370.370442
20	10.1695163	79.3839009	197.908861	370.386172
Ritz	10.1695239	79.3844233	197.910806	370.399134

STLM was used with a random starting vector and shifts derived from the corresponding Ritz values  $\Lambda_1, \Lambda_2, \Lambda_3, \Lambda_4$  estimating  $\lambda_1, \lambda_2, \lambda_3$ , and  $\lambda_4$ . For simplicity, full reorthogonalization was used. The sparse  $LU$  factorization needed by STLM was performed with the Harwell subroutine MA28. Calculations were performed on SUN SPARCstation 1<sup>+</sup> in double precision. The single biggest eigenvalue of  $(\mathcal{A} - \sigma\mathcal{B})^{-1}\mathcal{B}$  stabilized to full machine accuracy within 4 Lanczos steps, independent of  $N$ . It should be noted again that if we use zero shift, the number of Lanczos steps required exceeds half of the size of its computational matrix, i.e.  $(N + 1)^2 + 2(N + 2)(N + 3)$ , to get the same accuracy as nonzero shift has. In our model problem we have used Rayleigh-Ritz values when taking shifts. But if we have *a priori* knowledge of separation of eigenvalues of the given operator, we don't need to find upper bounds before computing lower bounds.

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