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Methods for computing lower bounds to eigenvalues of self-adjoint operators*

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Summary. New approaches for computing tight lower bounds to the eigenvalues of a class of semibounded self-adjoint operators are presented that require comparatively little *a priori* spectral information and permit the effective use of (among others) finite-element trial functions. A variant of the method of intermediate problems making use of operator decompositions having the form T^*T is reviewed and then developed into a new framework based on recent inertia results in the Weinstein-Aronszajn theory. This framework provides greater flexibility in analysis and permits the formulation of a final computational task involving sparse, well-structured matrices. Although our derivation is based on an intermediate problem formulation, our results may be specialized to obtain either the Temple-Lehmann method or Weinberger's matrix method.

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1. Introduction

Oftentimes the successful analysis of physical phenomena rests on the ability to closely bound the eigenvalues and eigenfunctions of differential operators. Frequently encountered examples include the prediction of resonant frequencies, vibrational mode shapes, and buckling loads of elastic structures; determination of bound state energy levels and associated electronic configurations for atoms and molecules; and computation of critical values of Reynolds numbers in viscous fluid flows. The related Hilbert space operators in such problems typically are

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semibounded below and self-adjoint, having eigenvalues of finite multiplicity below the lowest point of the essential spectra (if any exist).

Calculation of a bracketing interval that is guaranteed to contain a selected operator eigenvalue is equivalent to the computation of rigorous upper and lower bounds to that eigenvalue. While upper bounds are easily obtained by the Rayleigh-Ritz procedure (often manifested as the finite-element method), the computation of eigenvalue lower bounds is fundamentally more difficult and it is necessary to incorporate *a priori* spectral information that the Rayleigh-Ritz procedure does not require.

The Weinstein-Aronszajn intermediate problem methods are among the most flexible of the available techniques for obtaining these lower bound estimates. The original method was introduced by Weinstein in 1935 (cf. [36]) and provided a means of obtaining improvable lower bounds by incrementally tightening constraints. With the development of Aronszajn's extension in 1950 [1], the method of intermediate problems became much more widely applicable through the use of monotone sequences of quadratic forms.

The customary approach conceives of the original operator eigenvalue problem as a perturbation (generally large, possibly even relatively unbounded) of a simpler, resolvable, self-adjoint eigenvalue problem (the *base problem*) that provides rough lower bounds. The full perturbation is approximated systematically by related finite-rank perturbations producing eigenvalue problems that are intermediate between the base problem and the fully perturbed (unresolvable) eigenvalue problem. The associated intermediate eigenvalue estimates are obtained by computing the spectrum of the base operator summed with a positive semidefinite finite-rank operator that approximates the full perturbation. In conventional practice, this requires not only explicit knowledge of the reducing spaces and spectrum of the base operator but also special choices for the range space of the approximating finite-rank operator.

The primary computational task arising from the Weinstein-Aronszajn methods generally is a dense matrix eigenvalue problem that may be difficult to prepare and ultimately may impose heavy burdens on available computational resources. These practical obstructions are due primarily to the explicit involvement of the base problem eigenfunctions insofar as these functions have support throughout the problem domain and may be difficult to handle analytically. This fundamental difficulty has been effectively eliminated with methods we present here. Our work has elements in common with the earlier work of Weinberger [34, 35] and Gay [17], and follows up on a previous report by the second author [18] using techniques developed by the first author in [7].

After reviewing basic intermediate problem methods and recalling a useful variant (the method of second projection) in Sect. 2, we develop in Sect. 3 a computational approach that requires no eigenvector information from the base problem and only modest auxiliary information about the base operator spectrum. We also mention an alternative formulation that may be preferable in some circumstances. Section 4 contains a discussion of various monotonicity properties for the newly derived bounds and Sect. 5 explores the relationships with previ-

ously known methods. Section 6 touches upon some computational issues related to usage and provides illustrative examples.

2. Intermediate problem methods

2.1. Setting

Let $\mathfrak{H}$ be a separable complex Hilbert space with norm $\|u\|$ and inner product $\langle u, v\rangle$ (conjugate linear with respect to the first argument). Let A be a self-adjoint operator on a domain $\mathrm{Dom}(A)$ dense in $\mathfrak{H}$. We suppose that A is bounded below with spectrum that begins with isolated eigenvalues of finite multiplicity, $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_\infty \leq \infty$ and corresponding orthonormal eigenvectors u_1, u_2, etc. Here λ_∞ denotes the lowest limit point of the spectrum of A, that is, the first point of the essential spectrum. If A has compact resolvent then by convention we set $\lambda_\infty = \infty$. The closure of the quadratic form $\langle Au, u\rangle$ is denoted by $a(u)$ with an associated domain $\mathrm{Dom}(a) \supset \mathrm{Dom}(A)$. One may refer to Kato's excellent treatise [23] for basic results on quadratic forms in Hilbert spaces.

To apply the method of intermediate problems, it is necessary to have knowledge of a related eigenvalue problem

$$A_0 u = \lambda u \tag{2.1}$$

where A_0 is self-adjoint and bounded below on a domain $\mathrm{Dom}(A_0)$ dense in $\mathfrak{H}$, and $a_0(u) \leq a(u)$ for $u \in \mathrm{Dom}(a) \subset \mathrm{Dom}(a_0)$. The base problem (2.1), is assumed to have computable eigenvalues $\{\lambda_i^0\}$, such that $\lambda_1^0 \leq \lambda_2^0 \leq \ldots \leq \lambda_\infty^0 \leq \infty$ together with corresponding orthonormal eigenvectors u_1^0, u_2^0, etc. Consistent with previous notation, the lowest point of the essential spectrum of A_0 has been denoted λ_∞^0. The variational characterization for eigenvalues of self-adjoint operators implies that $\lambda_\infty^0 \leq \lambda_\infty$ and that for each i satisfying $\lambda_i < \lambda_\infty^0$, λ_i^0 exists and $\lambda_i^0 \leq \lambda_i$ [cf. 35]. In this way, the base problem provides lower bounds to the eigenvalues of A.

Unfortunately most suitable base problems (having *computable* eigenvalues and eigenvectors) produce very poor bounds, that are furthermore fixed and unimprovable. Intermediate problem methods provide an approach for adding back incrementally what was lost in passing from A to A_0. This is done in such a way so as to permit explicit resolution of the intermediate spectral problems – ultimately producing computable, improvable lower bounds to the eigenvalues of A. A thorough description of the ideas and techniques surrounding this approach may be found in [35, 36], and in the earlier review article [16]. We review one particular technique here – the method of second projection.

We assume in all that follows that $a(u)$ admits a decomposition as

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

where T is a closed operator from $\mathfrak{H}$ to a Hilbert space $\mathfrak{H}_*$ (equipped with inner product $\langle .,. \rangle_*$) and "$\subset$" here signifies that $a(u)$ is a closed restriction (not necessarily proper) of the form sum to the right.

2.2. An illustrative example

Let Ω be the unit cube in $\mathbb{R}^3$ and $\mathbf{u}(\mathbf{x}) = \{u_1(\mathbf{x}), u_2(\mathbf{x}), u_3(\mathbf{x})\}$ represent a vector-valued vector function defined for $\mathbf{x} \in \Omega$. For $\mathbf{u} \in (H^2(\Omega) \cap H_0^1(\Omega))^3$ and $\sigma > 0$, define the *Lamé operator*

$$A\mathbf{u} = -\Delta\mathbf{u} - \sigma\, \mathbf{grad}\, \mathbf{div}\, \mathbf{u}\ .$$

The operator A is densely defined in $\mathfrak{H} = L^2(\Omega)^3$ and self-adjoint on the domain of definition $\mathrm{Dom}\,(A) = [H^2(\Omega) \cap H_0^1(\Omega)]^3$ [24, p. 199]. The quadratic forms $a(\mathbf{u})$ and $a_0(\mathbf{u})$ are given by

$$a(\mathbf{u}) = \int_\Omega \left(\sum_{i,j=1}^{3} \left| \frac{\partial u_i}{\partial x_j} \right|^2 + \sigma \left| \sum_{i=1}^{3} \frac{\partial u_i}{\partial x_i} \right|^2 \right) dx_1 dx_2 dx_3$$

and

$$a_0(\mathbf{u}) = \int_\Omega \sum_{i,j=1}^{3} \left| \frac{\partial u_i}{\partial x_j} \right|^2 dx_1 dx_2 dx_3$$

respectively for $\mathbf{u} \in H_0^1(\Omega)^3 = \mathrm{Dom}\,(a) = \mathrm{Dom}\,(a_0)$. For $\mathbf{u} \in \mathrm{Dom}\,(a_0)$, define $T_0\mathbf{u} = \sqrt{\sigma}\, \mathbf{div}\, \mathbf{u}$. The operator T may then be defined as the closure of the operator T_0 with $\mathrm{Dom}\,(T) \supset H_0^1(\Omega)^3$ densely defined in $\mathfrak{H} = L^2(\Omega)^3$, mapping into $\mathfrak{H}_* = L^2(\Omega)$. Since $H_0^1(\Omega)^3$ is a core for T, the adjoint of T is directly computable as $T^* v = -\sqrt{\sigma}\, \mathbf{grad}\, v$ for $v \in H^1(\Omega)$. Note that the quadratic form $a_0(\mathbf{u})$ corresponds to the (resolvable) self-adjoint operator

$$A_0 = \begin{bmatrix} -\Delta & 0 & 0 \\ 0 & -\Delta & 0 \\ 0 & 0 & -\Delta \end{bmatrix} \begin{Bmatrix} u_1 \\ u_2 \\ u_3 \end{Bmatrix}$$

with $\mathrm{Dom}\,(A_0) = \mathrm{Dom}\,(A)$ as given above. A_0 has computable eigenvalues $\lambda_{ijk}^0 = (i^2 + j^2 + k^2)\pi^2$ with corresponding reducing subspaces $\mathfrak{U}_{ijk} = [\mathrm{span}\{v_{ijk}\}]^3$ where $v_{ijk} = \sin(i\pi x_1) \cdot \sin(j\pi x_2) \cdot \sin(k\pi x_3)$ for $i, j, k = 1, 2, \ldots$.

The eigenvalues of the Lamé operator are associated with the resonant frequencies of internal vibration that may be induced in a three-dimensional homogeneous isotropic elastic body (a cube in this case) having fixed boundary surfaces [19, Sect. 75]. The parameter σ may be expressed in terms of the Lamé moduli $\bar{\lambda}$ and $\bar{\mu}$ as $\sigma = (\bar{\lambda} + \bar{\mu})/\bar{\mu}$. $\bar{\mu}$ represents the shear modulus of the material while the modulus of compression is given by $\bar{\lambda} + \frac{2}{3}\bar{\mu}$ [19, Sect. 22]. As $\bar{\lambda}$ (and hence σ) increases, the material becomes progressively more resistant to compression. The limiting case $\bar{\lambda} \to \infty$ corresponds to incompressibility of the

material and is associated with the Stokes' eigenvalue problem [19, Sect. 58]: find nontrivial $\mathbf{u} \in [H^2(\Omega) \cap H_0^1(\Omega)]^3$ such that $-\Delta\mathbf{u} = \lambda\mathbf{u}$ and $\mathbf{div}\,\mathbf{u} = 0$. Note that the quadratic form for this problem is just the restriction of $a_0(\mathbf{u})$ to the subspace of divergence-free vector fields, $\mathfrak{M} = \{\mathbf{u} \in \mathfrak{H} | \mathbf{div}\ \mathbf{u} = 0\}$. Since $a_0|_{\mathfrak{M}} = a|_{\mathfrak{M}}$, the first monotonicity principle [35, Sect. 3.7] implies that the eigenvalues of the Lamé operator are lower bounds to the corresponding eigenvalues of the Stokes' eigenvalue problem for any finite value of $\sigma > 0$. This is of some practical significance itself since the smallest eigenvalue of the Stokes' eigenvalue problem plays a role in discerning stability of viscous incompressible fluid flows [22].

2.3. Intermediate problem construction

Returning to our development, we now select vectors $\{p_i\}_{i=1}^k \subset \mathrm{Dom}\,(T^*) \subset \mathfrak{H}_*$ and define the associated $\mathfrak{H}_*$-orthogonal projection

$$P_k u = \sum_{i,j=1}^{k} \langle u, p_i \rangle_* . \mathscr{B}_{ij} p_j$$

where $[.\mathscr{B}_{ij}]$ is the Moore–Penrose generalized matrix inverse to the Gram matrix $[\langle p_i, p_j \rangle_*]$. (One may refer to [32] for basic information relating to generalized matrix inverses.) In the linear elasticity problem just discussed, any vectors $\{p_i\}_{i=1}^k \subset H^1(\Omega)$ would be admissable.

Define the quadratic form

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

for all u in $\mathrm{Dom}\,(a_0) \cap \mathrm{Dom}\,(T)$. Since $\mathrm{Ran}\,(P_k) \subset \mathrm{Dom}\,(T^*)$, $P_k T$ may be extended by continuity to all of $\mathfrak{H}$ and $a_k(u)$ may be associated with a self-adjoint operator given by

$$A_k = A_0 + \sum_{i,j=1}^{k} \langle \cdot, T^* p_i \rangle . \mathscr{B}_{ij} T^* p_j \supset A_0 + T^* P_k T , \tag{2.2}$$

with $\mathrm{Dom}\,(A_k) = \mathrm{Dom}\,(A_0)$. The eigenvalues of A_k may be denoted analogously to those of A_0 and A as $\lambda_1^{(k)} \le \lambda_2^{(k)} \le \ldots \le \lambda_\infty^{(k)} \le \infty$. Because $a_0(u) \le a_k(u) \le a_{k+1}(u) \le a(u)$ for all $u \in \mathrm{Dom}\,(a)$, the eigenvalues of A_k lie intermediate between those of A_0 and those of A, and are monotone increasing in k, the dimension of the projecting subspace. That is,

$$\lambda_i^0 \le \lambda_i^{(k)} \le \lambda_i^{(k+1)} \le \lambda_i$$

for each i such that $\lambda_i < \lambda_\infty^0$.

The finite-rank nature of the perturbation to A_0 expressed in (2.2) permits computation of $\{\lambda_i^{(k)}\}$ through consideration of the rank and inertia of the *Weinstein-Aronszajn (W-A) matrix*,

$$\mathscr{W}_k(\lambda) = [\langle p_i, p_j\rangle_* + \langle R_\lambda^0 T^* p_i, T^* p_j\rangle] \,, \tag{2.3}$$

considered as a function of the eigenvalue parameter λ. Here R_λ^0 denotes the resolvent operator $(A_0 - \lambda)^{-1}$. We introduce the following notation:

$N(\lambda)$ is the number of eigenvalues of A strictly less than the parameter λ,
$N_k(\lambda)$ is the number of eigenvalues of A_k strictly less than the parameter λ,
$N_0(\lambda)$ is the number of eigenvalues of A_0 strictly less than the parameter λ,
$\mathbb{D}^-[.\mathscr{M}]$ is the negative inertia of a Hermitian matrix $.\mathscr{M}$
(i.e., the number of negative eigenvalues of $.\mathscr{M}$), and
$\operatorname{null}[.\mathscr{M}]$ is the nullity of a square matrix $.\mathscr{M}$.

The following extension of the spectrum-slicing formulas of [7] is developed in the appendix.

$$N(\lambda) \le N_k(\lambda) = N_0(\lambda) - \{\operatorname{null}[\mathscr{W}_k(\lambda)] + \mathbb{D}^-[\mathscr{W}_k(\lambda)]\} + \operatorname{null}[\langle p_i, p_j\rangle_*] \tag{2.4}$$

for any $\lambda \le \lambda_\infty^0$ at which $\mathscr{W}_k(\lambda)$ is defined. Provided that it is possible to evaluate $\mathscr{W}_k(\lambda)$ for any such λ, (2.4) may be used directly to isolate and locate eigenvalues of A_k to any degree of accuracy desired (at least in principle), thus providing lower bounds to the corresponding eigenvalues of A.

Additional knowledge of $\operatorname{Ker}(T^*)$ may be incorporated to further improve these bounds. Specifically, suppose we know of ω linearly independent vectors $\{z_i\}_{i=1}^{\omega} \subset \operatorname{Ker}(T^*)$ and consider the effect of removing from $\{p_i\}_{i=1}^{k}$ components lying in $\operatorname*{span}_{i=1,\ldots,\omega}(z_i)$:

$$\tilde{p}_i = p_i - \sum_{l,m=1}^{\omega} \langle p_i, z_l\rangle_* \mathscr{Z}_{lm} z_m \,, \tag{2.5}$$

where $[\mathscr{Z}_{lm}]$ is the matrix inverse to $[\langle z_l, z_m\rangle_*]$. Note that relative to the natural partial ordering of Hermitian matrices,

$$[\langle p_i, p_j\rangle_*] = [\langle \tilde{p}_i, \tilde{p}_j\rangle_* + \sum_{l,m=1}^{\omega} \langle p_i, z_l\rangle_* \mathscr{Z}_{lm} \langle z_m, p_j\rangle_*] \ge [\langle \tilde{p}_i, \tilde{p}_j\rangle_*] \,.$$

So, defining $[.\tilde{\mathscr{B}}_{ij}]$ to be the Moore–Penrose generalized inverse of the Gram matrix $[\langle \tilde{p}_i, \tilde{p}_j\rangle_*]$, we have that $[.\tilde{\mathscr{B}}_{ij}] \ge [.\mathscr{B}_{ij}]$ and

$$A_k \le A_0 + \sum_{i,j=1}^{k} \langle \cdot, T^* \tilde{p}_i\rangle . \tilde{\mathscr{B}}_{ij} T^* \tilde{p}_j \le A \,. \tag{2.6}$$

The associated W-A matrix may be expressed directly in terms of $\{p_i\}_{i=1}^{k}$ as

$$\mathscr{W}_k^{\omega}(\lambda) = [\langle p_i, p_j\rangle_* - \sum_{l,m=1}^{\omega} \langle p_i, z_l\rangle_* \mathscr{Z}_{lm} \langle z_m, p_j\rangle_* + \langle R_\lambda^0 T^* p_i, T^* p_j\rangle] \,. \tag{2.7}$$

Augment the projecting vectors $\{p_i\}_{i=1}^k$ by defining $p_{k+j} = z_j$ for $j = 1, \ldots, \omega$ and let $\mathscr{W}_{k+\omega}^{\cdot}(\lambda)$ denote the corresponding W-A matrix obtained from (2.3). Note that $[\langle z_l, z_m\rangle_*]$ is positive definite and appears as the lower $\omega \times \omega$ principal submatrix of $\mathscr{W}_{k+\omega}^{\cdot}(\lambda)$, so one may see from (2.7) that $\mathscr{W}_k^{\cdot\omega}(\lambda)$ is the Schur complement of $[\langle z_l, z_m\rangle_*]$ in $\mathscr{W}_{k+\omega}^{\cdot}(\lambda)$ (cf. [20]). Using the additivity of inertia over Schur complementation we find

$$\text{null}\,[\mathscr{W}_{k+\omega}^{\cdot}(\lambda)] + \mathbb{D}^-[\mathscr{W}_{k+\omega}^{\cdot}(\lambda)] = \text{null}\,[\mathscr{W}_k^{\cdot\omega}(\lambda)] + \mathbb{D}^-[\mathscr{W}_k^{\cdot\omega}(\lambda)]\ .$$

Thus from the spectrum-slicing formula (2.4) we see that the bounds obtained by reducing the kernel of T^* by $\underset{i=1,\ldots,\omega}{\text{span}}\,(z_i)$ as in (2.7) are identical to what would be obtained by simply augmenting the original projecting set $\{p_i\}_{i=1}^k$ with $\{z_j\}_{j=1}^\omega$. While the form of (2.7) may hold some practical advantages in computational strategies that make direct use of the W-A matrix (e.g., [8]), we may omit any explicit reference to the reduction of $\text{Ker}\,(T^*)$ with no loss of generality and henceforth consider only (2.3).

For general choices of projecting vectors $\{p_i\}$, note that the evaluation of $\mathscr{W}_k^{\cdot}(\lambda)$ is very difficult because the action of R_λ^0 is rarely accessible in a sufficiently accurate, computationally usable form. Bazley and Fox [5] proposed the use of a "special choice", determining vectors $\{p_i\}_{i=1}^k$ so that $T^*p_i = u_i^0$. Although this choice for $\{p_i\}$ makes evaluation of $\mathscr{W}_k^{\cdot}(\lambda)$ comparatively straightforward, one is left with a highly constrained choice of the projecting vectors $\{p_i\}$ and also the (possibly) onerous task of solving the many operator equations, $T^*p_i = u_i^0$. To circumvent some of these difficulties Bazley and Fox introduced the method of second projection.

Following [5], let us define for some fixed $\delta \neq 0$, $B_k = T^*P_kT + \delta^2 I$. The operator B_k is bounded, self-adjoint, and positive definite. Furthermore, it has an explicit inverse given by

$$B_k^{-1}v = \frac{1}{\delta^2}[v - \sum_{\ell,m=1}^{k} \langle v, T^*p_\ell\rangle \mathscr{C}_{\ell m} T^*p_m] \tag{2.8}$$

where $[\mathscr{C}_{\ell m}]$ is the Moore–Penrose generalized matrix inverse to $[\delta^2\langle p_i, p_j\rangle_* + \langle T^*p_i, T^*p_j\rangle]$.

Upon choosing a set of vectors $\{\hat{p}_i\}_{i=1}^n$, we may define a projection onto $\underset{i=1,\ldots,n}{\text{span}}\,\{\hat{p}_i\}$, orthogonal with respect to the inner product induced by B_k:

$$\hat{P}_n = \sum_{i,j=1}^{n} \langle \cdot, B_k\hat{p}_i\rangle)\mathscr{S}_{ij}\hat{p}_j$$

where now $[\mathscr{S}_{ij}]$ is the Moore–Penrose generalized matrix inverse to $[\langle B_k\hat{p}_i, \hat{p}_j\rangle]$. lt is easy to see then that $B_k\hat{P}_n$ is a bounded, symmetric, positive semidefinite operator, and that $\langle B_k\hat{P}_n u, u\rangle \leq \langle B_k u, u\rangle$ for all $u \in \mathfrak{H}$. Thus, if we define

$$A_{k,n} = A_0 - \delta^2 + B_k\hat{P}_n\ , \tag{2.9}$$

it is clear that the eigenvalues of $A_{k,n}$ form lower bounds to the corresponding eigenvalues of A and that they are monotone increasing in both k and n. The associated $n \times n$ W-A matrix is given by

$$\mathscr{W}_{k,n}^{\cdot}(\lambda) = [\langle \hat{p}_i + R^0_{\lambda+\delta^2} B_k \hat{p} i, B_k \hat{p}_j \rangle] \tag{2.10}$$

This matrix will be pivotal in our later development. The corresponding counting function, $N_{k,n}(\lambda)$ satisfies

$$\begin{aligned} N(\lambda) &\le N_{k,n}(\lambda) \\ &= N_0(\lambda + \delta^2) - \{\text{null}\,[\mathscr{W}_{k,n}^{\cdot}(\lambda)] + \mathbb{D}^-[\mathscr{W}_{k,n}^{\cdot}(\lambda)]\} + \text{null}\,[\langle \hat{p}_i, \hat{p}_j \rangle] \end{aligned} \tag{2.11}$$

for each $\lambda < \lambda^0_\infty$ where $\mathscr{W}_{k,n}^{\cdot}(\lambda)$ is well defined.

Now, if we were to choose the vectors $\{\hat{p}_i\}_{i=1}^n$ so that $\hat{p}_i = B_k^{-1} u_i^0$, then the W-A matrix (2.10) would be explicitly computable as

$$\mathscr{W}_{k,n}^{\cdot}(\lambda) = \left[\left(\frac{1}{\delta^2} + \frac{1}{\lambda_i^0 - (\lambda + \delta^2)} \right) \delta_{ij} - \frac{1}{\delta^2} \sum_{\ell,m=1}^{k} \langle u_i^0, T^* p_\ell \rangle \mathscr{C}_{\ell m} \langle T^* p_m, u_j^0 \rangle \right] \tag{2.12}$$

(δ_{ij} denotes the Kronecker delta). Since $A_{k,n}$ as defined in (2.9) would then have the explicitly known finite-dimensional reducing space $\underset{i=1,\ldots,n}{\text{span}}\,\{u_i^0\}$, the computational task associated with (2.12) could be refashioned into a linear $n \times n$ matrix eigenvalue problem –

$$[\text{diag}\,(\lambda_i^0 - \delta^2) + \mathscr{D}]\mathbf{x} = \lambda \mathbf{x}\,.$$

Note that $\mathscr{D}$ here is the matrix inverse to $[\langle u_i^0, B_k^{-1} u_j^0 \rangle]$ which will in nearly every case of interest *not* be sparse because the eigenvectors $\{u_i^0\}$ will have support throughout the problem domain.

It was observed in [4] that the lower bound for the νth eigenvalue derived from (2.9) improves monotonically as $|\delta|$ increases until it reaches the value $\lambda^0_{n+1} - \delta^2$ at which point the bound begins to deteriorate as $|\delta|$ increases further. Thus, the optimum value of δ with which to estimate λ_ν is attained when $\delta^2 = \lambda^0_{n+1} - \lambda_\nu^{(k,n)}$, though of course this value is not generally known at the outset. Börsch-Supan [12] showed that this optimum bound is achieved (simultaneously for every $\nu \le n$) with the *method of truncation* [3], which makes use of the same information as the method of second projection but involves instead the resolution of a (dense) matrix eigenvalue problem of larger dimension $n + k$.

3. Extensions

3.1. An eigenvector-free formulation

In the previous discussion of Weinstein-Aronszajn methods, the strategy implicit in utilizing the formula (2.10), involves *fixing* a nonzero constant δ, *fixing* families

of projecting vectors $\{p_i\}_{i=1}^k$ or $\{\hat{p}_i\}_{i=1}^n$ (generally through a "special choice") and then *varying* λ to obtain the best possible lower bound – either by finding a value for which $\mathscr{W}(\lambda)$ loses rank or by resolving an equivalent (dense) matrix eigenvalue problem. This approach depends on the availability of base problem eigenvectors in general since there is little other possibility of adequately treating the resolvent operator, R_λ^0, involved in the W-A matrix. In this section, we remove the debilitating dependence on eigenvectors and in so doing allow more flexibility in the selection of projecting vectors.

Returning to the W-A matrix (2.10) associated with the method of second projection, we define $\mu = \lambda + \delta^2$ and then consider only those λ for which $\lambda < \mu$. Introduce the change of variable $q_i = R_\mu^0 B_k \hat{p}_i$ into (2.10) to get

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

which may be further simplified with the aid of (2.8) to get

$$\begin{aligned}\mathscr{W}_{k,n}(\lambda) &= [\langle q_i, (A_0 - \mu)q_j\rangle + \frac{1}{\mu - \lambda}\{\langle (A_0 - \mu)q_i, (A_0 - \mu)q_j\rangle \\ &\quad - \sum_{\ell,m=1}^{k} \langle (A_0 - \mu)q_i, T^* p_\ell\rangle C_{\ell m} \langle T^* p_m, (A_0 - \mu)q_j\rangle\}] \qquad (3.1)\end{aligned}$$

Fix μ, $\{q_i\}_{i=1}^n \subset \mathrm{Dom}\,(A_0)$, and $\{p_i\}_{i=1}^k \subset \mathrm{Dom}\,(T^*)$ and observe that $\mathscr{W}_{k,n}(\lambda)$ will be the W-A matrix for an intermediate problem for each (fixed) $\lambda < \mu$, however as λ changes, δ^2 changes, $\{\hat{p}_i\}$ changes, $[\mathscr{C}_{\ell m}]$ changes, thus the related intermediate problem changes as well, and not at all in a monotonic fashion. By using the spectrum-slicing formula (2.11), we may still interpret each $\lambda < \mu$ as a lower bound to an eigenvalue λ_p of A, with index $p = N_0(\mu) - \{\mathrm{null}\,[\mathscr{W}_{k,n}(\lambda)\rangle] + \mathbb{D}^-[\mathscr{W}_{k,n}(\lambda)]\} + 1$. Finding the best lower bound to λ_p for fixed μ, fixed $\{q_i\}$, and fixed $\{p_i\}$ would then involve finding the largest λ that leaves $\{\mathrm{null}\,\mathscr{W}_{k,n}(\lambda)] + \mathbb{D}^-[\mathscr{W}_{k,n}(\lambda)]\}$ unchanged. At first glance, the computational task one now faces appears to involve constrained nonlinear programming and so may not be any more appealing than previous methods. However, a slight reformulation will be seen to produce a well-structured linear matrix eigenvalue problem. Define the matrices:

$$\begin{aligned}\mathscr{F}_1 &= [\langle q_i, (A_0 - \mu)q_j\rangle] \in \mathbb{C}^{n\times n} ,\\ \mathscr{F}_2 &= [\langle p_i, p_j\rangle_*] \in \mathbb{C}^{k\times k} ,\\ \mathscr{G}_1 &= [\langle (A_0 - \mu)q_i, (A_0 - \mu)q_j\rangle] \in \mathbb{C}^{n\times n} ,\\ \mathscr{G}_2 &= [\langle T^* p_i, T^* p_j\rangle] \in \mathbb{C}^{k\times k} ,\end{aligned}$$

and

$$\mathscr{H} = [\langle (A_0 - \mu)q_i, T^* p_j\rangle] \in \mathbb{C}^{n\times k} .$$

Using "†" to denote a Moore–Penrose generalized inverse, the W-A matrix $\mathscr{W}_{k,n}(\lambda)$ of (3.1) may be compactly expressed as

$$\mathscr{W}_{k,n}(\lambda) = \mathscr{F}_1 + \frac{1}{\mu - \lambda}\{\mathscr{G}_1 - \mathscr{H}[(\mu - \lambda)\mathscr{F}_2 + \mathscr{G}_2]^\dagger \mathscr{H}^*\} .$$

Defining the matrix pencil

$$\mathscr{M}_{k,n}(\zeta) = \begin{bmatrix} \mathscr{T}_1 & 0 \\ 0 & \mathscr{T}_2 \end{bmatrix} - \zeta \begin{bmatrix} \mathscr{G}_1 & \mathscr{H} \\ \mathscr{H}^* & \mathscr{G}_2 \end{bmatrix}, \tag{3.2}$$

we find for $\zeta = (\lambda - \mu)^{-1}$

$$\mathscr{W}_{k,n}(\lambda) = [.\mathscr{M}_{k,n}(\zeta)/(.\mathscr{T}_2 - \zeta\mathscr{G}_2)] ,$$

signifying the (generalized) Schur complement of $.\mathscr{M}_{k,n}(\zeta)$ with respect to $\mathscr{T}_2 - \zeta\mathscr{G}_2$ [15]. Note that the matrix $\begin{bmatrix} \mathscr{G}_1 & \mathscr{H} \\ \mathscr{H}^* & \mathscr{G}_2 \end{bmatrix}$ is positive semidefinite, being the Gram matrix of the vectors $\{(A_0 - \mu)q_i\}_{i=1}^n$ and $\{T^* p_j\}_{j=1}^k$. Using the additivity of inertia over Schur complementation [15] we find

$$\begin{aligned} \operatorname{null}[\mathscr{W}_{k,n}(\lambda)] + \mathbb{D}^-[\mathscr{W}_{k,n}(\lambda)] &= \operatorname{null}[.\mathscr{M}_{k,n}(\zeta)] + \mathbb{D}^-[.\mathscr{M}_{k,u}(\zeta)] \\ &\quad - \{\operatorname{null}[.\mathscr{T}_2 - \zeta.\mathscr{G}_2] + \mathbb{D}^-[.\mathscr{T}_2 - \zeta.\mathscr{G}_2]\} . \end{aligned}$$

Since $\lambda < \mu$ implies $\zeta < 0$, $\mathscr{T}_2 - \zeta\mathscr{G}_2$ is positive semi-definite so that $\mathbb{D}^-[.\mathscr{T}_2 - \zeta.\mathscr{G}_2] = 0$ and $\operatorname{null}[.\mathscr{T}_2 - \zeta.\mathscr{G}_2] = \operatorname{null}[.\mathscr{T}_2]$. Furthermore, $\operatorname{null}[\langle \hat{p}_i, \hat{p}_j \rangle] = \operatorname{null}[\langle B_k\hat{p}_i, B_k\hat{p}_j \rangle] = \operatorname{null}[.\mathscr{G}_1]$. Thus from (2.11) we have

$$N(\lambda) \le N_0(\mu) - \{\operatorname{null}[.\mathscr{M}_{k,n}(\zeta)] + \mathbb{D}^-[.\mathscr{M}_{k,n}(\zeta)\} + \operatorname{null}[.\mathscr{G}_1] + \operatorname{null}[.\mathscr{T}_2] . \tag{3.3}$$

3.2. A generalized matrix eigenvalue problem

Evidently, the critical points of $\operatorname{null}[.\mathscr{M}_{k,n}(\zeta)] + \mathbb{D}^-[.\mathscr{M}_{k,n}(\zeta)]$ occur at the eigenvalues of the generalized matrix eigenvalue problem

$$\begin{bmatrix} \mathscr{T}_1 & 0 \\ 0 & \mathscr{T}_2 \end{bmatrix} \begin{Bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{Bmatrix} = \zeta \begin{bmatrix} \mathscr{G}_1 & \mathscr{H} \\ \mathscr{H}^* & \mathscr{G}_2 \end{bmatrix} \begin{Bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{Bmatrix} \tag{3.4}$$

We recall the following

Definition 3.1. Let $.\mathscr{A}$ and $.\mathscr{B} \in \mathbb{C}^{m\times m}$ be Hermitian matrices with $.\mathscr{B}$ positive semidefinite. ζ is called a *discrete eigenvalue* of the problem

$$.\mathscr{A}\mathbf{x} = \zeta.\mathscr{B}\mathbf{x}$$

if $\nu(\zeta) > 0$ where

$$\nu(\zeta) \stackrel{\text{def}}{=} \dim\{\mathbf{x} \in \mathbb{C}^m \,|\, .\mathscr{A}\mathbf{x} = \zeta.\mathscr{B}\mathbf{x} \text{ and } \mathbf{x}^*\mathbf{y} = 0 \text{ for all } \mathbf{y} \in \operatorname{Ker}.\mathscr{A} \cap \operatorname{Ker}.\mathscr{B}\} .$$

$\nu(\zeta)$ is then called the *multiplicity* of the eigenvalue ζ. By convention,

$$\nu(\infty) = \dim \operatorname{Ker}(.\mathscr{B}) \setminus \operatorname{Ker}(.\mathscr{A})$$

is the multiplicity of "the eigenvalue at infinity".

Thus the eigenvalues of (3.4) may or may not be discrete, and if discrete, may be finite or infinite, all depending on the relative orientation of the kernels of the left- and right-hand matrices, (cf. [31]). Notice there can only be a finite number of discrete eigenvalues (including the eigenvalue at infinity). However, since $\mathrm{Ker}\,\mathscr{F}_2 \subset \mathrm{Ker}\,\mathscr{G}_2 \subset \mathrm{Ker}\,\mathscr{H}$, $\mathrm{Ker}\,\mathscr{G}_1 \subset \mathrm{Ker}\,\mathscr{H}^*$ and $\mathrm{Ker}\,\mathscr{G}_1 \subset \mathrm{Ker}\,\mathscr{F}_1$, one may observe that $\mathrm{Ker}\,\mathscr{G}_1 \oplus \mathrm{Ker}\,\mathscr{F}_2 = \mathrm{Ker}\left(\begin{bmatrix}\mathscr{F}_1 & 0\\ 0 & \mathscr{F}_2\end{bmatrix}\right) \cap \mathrm{Ker}\left(\begin{bmatrix}\mathscr{G}_1 & \mathscr{H}\\ \mathscr{H}^* & \mathscr{G}_2\end{bmatrix}\right)$. Any $x_1 \in \mathrm{Ker}\,\mathscr{G}_1$ and $x_2 \in \mathrm{Ker}\,\mathscr{F}_2$ would trivially satisfy (3.4) for every finite value of ζ.

Excluding trivial cases, (3.4) will have discrete (finite) eigenvalues which we label as

$$\zeta_1 \le \zeta_2 \le \ldots \le \zeta_\ell < 0 \le \zeta_{\ell+1} \le \cdots,$$

($\ell = 0$ when all are non-negative or infinite). For a given index r, fix μ so that $\lambda^0_{r-1} < \mu \le \lambda^0_r$. If $\mathrm{Ker}\left(\begin{bmatrix}\mathscr{G}_1 & \mathscr{H}\\ \mathscr{H}^* & \mathscr{G}_2\end{bmatrix}\right) \subset \mathrm{Ker}\left(\begin{bmatrix}\mathscr{F}_1 & 0\\ 0 & \mathscr{F}_2\end{bmatrix}\right)$, then all discrete eigenvalues are finite and for any eigenvalue ζ_p with $p \le \ell$ we have from (3.3)

$$N\left(\mu + \frac{1}{\zeta_p}\right) \le r - 1 - \{\mathbb{D}^-[\mathscr{M}_{k,n}(\zeta_p)] + (\mathrm{null}[\mathscr{M}_{k,n}(\zeta_p)] - \mathrm{null}[\mathscr{G}_1] - \mathrm{null}[\mathscr{F}_2])\} = r - 1 - m(p)$$

where $m(p) = \max\{m | \zeta_m = \zeta_p\}$. Thus for any matrix eigenvalue ζ_p with $p \le \ell$, we have a corresponding lower bound to an eigenvalue of A:

$$\mu + \frac{1}{\zeta_p} \le \lambda_{r-m(p)} \le \lambda_{r-p}$$

On the other hand, if $\mathrm{Ker}\left(\begin{bmatrix}\mathscr{G}_1 & \mathscr{H}\\ \mathscr{H}^* & \mathscr{G}_2\end{bmatrix}\right) \not\subset \mathrm{Ker}\left(\begin{bmatrix}\mathscr{F}_1 & 0\\ 0 & \mathscr{F}_2\end{bmatrix}\right)$, then there will be infinite eigenvalues of (3.4) that may confound the association between the inertia of $\mathscr{M}_{k,n}(\zeta_p)$ and the eigenvalue index p.

We consider this issue in a wider context of generalized Hermitian matrix eigenvalue problems.

Lemma 3.2. *Let $\mathscr{A}$ and $\mathscr{B} \in \mathbb{C}^{m\times m}$ be Hermitian matrices with $\mathscr{B}$ positive semidefinite. Choose $\eta \in \mathbb{R}$ and let p be the number of discrete eigenvalues of $A\mathbf{x} = \zeta B\mathbf{x}$ contained in the interval $(-\infty, \eta]$. Further, let $\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_\gamma\}$ be a basis for $\mathrm{Ker}\,(\mathscr{B})$ and define $\mathscr{C} = [c_{ij}] \in \mathbb{C}^{\gamma\times\gamma}$ by $c_{ij} = \mathbf{v}_i^* \mathscr{A}\mathbf{v}_j$ for $i, j = 1, \ldots \gamma$. Then*

$$\mathrm{null}\,[\mathscr{A} - \eta\mathscr{B}] + \mathbb{D}^-[\mathscr{A} - \eta\mathscr{B}] = p + \mathrm{null}\,[\mathscr{C}] + \mathbb{D}^-[\mathscr{C}]$$

Proof. Let $\mathscr{V} \in \mathbb{C}^{m\times\gamma}$ have columns $\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_\gamma\}$ and let the columns of $\overline{\mathscr{V}} \in \mathbb{C}^{m\times(m-\gamma)}$ form a basis for $[\mathrm{Ker}\,(\mathscr{B})]^\perp$. Define the parameterized matrices $\mathscr{M}_\tau = \mathscr{A} + (\tau - \eta)\mathscr{B}$ and $\mathscr{Z}_\tau = [\mathscr{V}\ \frac{1}{\sqrt{\tau}}\overline{\mathscr{V}}]$. Then $\mathscr{Z}_\tau$ is nonsingular for each $\tau > 0$ and

$$\mathscr{Z}_\tau^*\mathscr{M}_\tau\mathscr{Z}_\tau = \begin{bmatrix} \mathscr{C} & \frac{1}{\sqrt{\tau}}\mathscr{V}^*\mathscr{A}\overline{\mathscr{V}} \\ \frac{1}{\sqrt{\tau}}\overline{\mathscr{V}}^*\mathscr{A}\mathscr{V} & \overline{\mathscr{V}}^*\mathscr{B}\overline{\mathscr{V}} + \frac{1}{\sqrt{\tau}}\overline{\mathscr{V}}^*(\mathscr{A}-\eta\mathscr{B})\overline{\mathscr{V}} \end{bmatrix}.$$

If $\mathscr{C}$ is nonsingular then $\dim[\mathrm{Ker}(\mathscr{A}) \cap \mathrm{Ker}(\mathscr{B})] = 0$ and, since $\overline{\mathscr{V}}^*\mathscr{B}\overline{\mathscr{V}}$ is positive definite, $\mathbb{D}^-[\mathscr{M}_\tau] = \mathbb{D}^-[\mathscr{C}]$, for all $\tau > T$, with sufficiently large $T > 0$. If $\mathscr{C}$ is singular, we are free to pick an orthonormal basis for $\mathrm{Ker}(\mathscr{B})$ that constitute the columns of $\mathscr{V} = [\mathscr{V}_1\mathscr{V}_2]$, so that $\mathscr{C} = \mathscr{V}^*\mathscr{A}\mathscr{V} = \begin{bmatrix} 0 & 0 \\ 0 & \mathscr{C}_2 \end{bmatrix}$, and $\mathscr{C}_2 = \mathscr{V}_2^*\mathscr{A}\mathscr{V}_2$, is nonsingular. This produces a natural partitioning of $\mathscr{Z}_\tau^*\mathscr{M}_\tau\mathscr{Z}_\tau$ as

$$\mathscr{Z}_\tau^*\mathscr{M}_\tau\mathscr{Z}_\tau = \begin{bmatrix} 0 & 0 & \frac{1}{\sqrt{\tau}}\mathscr{V}_1^*\mathscr{A}\overline{\mathscr{V}} \\ 0 & \mathscr{C}_2 & \frac{1}{\sqrt{\tau}}\mathscr{V}_2^*\mathscr{A}\overline{\mathscr{V}} \\ \frac{1}{\sqrt{\tau}}\overline{\mathscr{V}}^*\mathscr{A}\mathscr{V}_1 & \frac{1}{\sqrt{\tau}}\overline{\mathscr{V}}^*\mathscr{A}\mathscr{V}_2 & \overline{\mathscr{V}}^*\mathscr{B}\overline{\mathscr{V}} + \frac{1}{\tau}\overline{\mathscr{V}}^*(\mathscr{A}-\eta\mathscr{B})\overline{\mathscr{V}} \end{bmatrix}.$$

For any vector $y \in \mathrm{Ker}(\overline{\mathscr{V}}^*\mathscr{A}\mathscr{V}_1)$, observe

$$\mathscr{A}\mathscr{V}_1 y = \mathscr{M}_\tau\mathscr{Z}_\tau \begin{Bmatrix} y \\ \mathbf{0} \\ \mathbf{0} \end{Bmatrix} = (\mathscr{Z}_\tau^*)^{-1}\mathscr{Z}_\tau^*\mathscr{M}_\tau\mathscr{Z}_\tau \begin{Bmatrix} y \\ \mathbf{0} \\ \mathbf{0} \end{Bmatrix} = 0\,.$$

Thus $\mathscr{V}_1$ is an injective mapping from $\mathrm{Ker}(\overline{\mathscr{V}}^*\mathscr{A}\mathscr{V}_1)$ into $\mathrm{Ker}(\mathscr{A}) \cap \mathrm{Ker}(\mathscr{B})$. Furthermore, for any vector $x \in \mathrm{Ker}(\mathscr{A}) \cap \mathrm{Ker}(\mathscr{B})$, $x = \mathscr{V}_1 y + \mathscr{V}_2 z$ for some pair of vectors y and z. But then $0 = \mathscr{V}_2^*\mathscr{A}x = \mathscr{C}_2 z$ which implies that $z = 0$. Thus $y \in \mathrm{Ker}(\overline{\mathscr{V}}^*\mathscr{A}\mathscr{V}_1)$ and $\mathscr{V}_1$ is a bijection between $\mathrm{Ker}(\overline{\mathscr{V}}^*\mathscr{A}\mathscr{V}_1)$ and $\mathrm{Ker}(\mathscr{A}) \cap \mathrm{Ker}(\mathscr{B})$. This in turn implies that $\mathrm{null}(\overline{\mathscr{V}}^*\mathscr{A}\mathscr{V}_1) = \dim(\mathrm{Ker}(\mathscr{A}) \cap \mathrm{Ker}(\mathscr{B}))$ and $\mathrm{rank}(\overline{\mathscr{V}}^*\mathscr{A}\mathscr{V}_1) = \mathrm{null}(\mathscr{C}) - \dim(\mathrm{Ker}(\mathscr{A}) \cap \mathrm{Ker}(\mathscr{B}))$. Now define the block Gauss transformations,

$$\mathscr{N}_1 = \begin{bmatrix} I & 0 & 0 \\ 0 & I & 0 \\ \frac{1}{\sqrt{\tau}}\mathscr{E}_1 & 0 & I \end{bmatrix} \quad \text{and} \quad \mathscr{N}_2 = \begin{bmatrix} I & 0 & 0 \\ 0 & I & \frac{1}{\sqrt{\tau}}\mathscr{E}_2 \\ 0 & 0 & I \end{bmatrix},$$

where $\mathscr{E}_1 = -\mathscr{G}(\tau)^{-1}\overline{\mathscr{V}}^*\mathscr{A}\mathscr{V}_1$ with $\mathscr{G}(\tau) = \overline{\mathscr{V}}^*\mathscr{B}\overline{\mathscr{V}} + \frac{1}{\tau}\mathscr{V}^*(\mathscr{A}-\eta\mathscr{B})\overline{\mathscr{V}} - \frac{1}{\tau}\mathscr{E}_2^*\mathscr{C}_2\mathscr{E}_2$, and $\mathscr{E}_2 = -\mathscr{C}_2^{-1}\mathscr{V}_2^*\mathscr{A}\overline{\mathscr{V}}$. Notice that $\mathscr{G}(\tau)$ is positive definite for all $\tau > T$ with sufficiently large $T > 0$, hence $\mathscr{N}_1$ and $\mathscr{N}_2$ will be invertible for all $\tau > T$. A straightforward calculation shows that $\mathscr{N}_1^*\mathscr{N}_2^*(\mathscr{Z}_\tau^*\mathscr{M}_\tau\mathscr{Z}_\tau)\mathscr{N}_1\mathscr{N}_2 = \mathrm{diag}[-\mathscr{E}_1^*\mathscr{G}(\tau)\mathscr{E}_1, \mathscr{C}_2, \mathscr{G}(\tau)]$. Hence for all $\tau > T$ with $T > 0$ sufficiently large, we find

$$\begin{aligned} \mathbb{D}^-[\mathscr{M}_\tau] &= \mathbb{D}^-[-\mathscr{E}_1^*\mathscr{G}(\tau)\mathscr{E}_1] + \mathbb{D}^-[\mathscr{C}_2] \\ &= \mathrm{rank}[\mathscr{E}_1] + \mathbb{D}^-[\mathscr{C}] \\ &= \mathrm{null}[\mathscr{C}] + \mathbb{D}^-[\mathscr{C}] - \dim(\mathrm{Ker}(\mathscr{A}) \cap \mathrm{Ker}(\mathscr{B}))\,. \end{aligned}$$

Now let $\mathscr{U}$ be a matrix with orthonormal columns that span $[\mathrm{Ker}(\mathscr{A}) \cap \mathrm{Ker}(\mathscr{B})]^\perp$. Then $\mathbb{D}^-[\mathscr{M}_\tau] = \mathbb{D}^-[\mathscr{U}^*\mathscr{M}_\tau\mathscr{U}]$ for all τ and $\mathscr{U}^*\mathscr{M}_\tau\mathscr{U}$ is

singular if and only if $\eta - \tau$ is a discrete eigenvalue of $.\mathscr{A}\mathbf{x} = \zeta.\mathscr{B}\mathbf{x}$. Since $.\mathscr{B}$ is positive semidefinite, the eigenvalues of $\mathscr{U}^*.\mathscr{M}_\tau\mathscr{U}$ are evidently continuous and monotone nondecreasing as functions of τ. Furthermore, since $\det(\mathscr{U}^*.\mathscr{M}_\tau\mathscr{U})$ is analytic in τ and not identically zero, any negative eigenvalue of $\mathscr{U}^*.\mathscr{M}_\tau\mathscr{U}$ that reaches zero must cross from negative to positive at that point. Hence as τ increases in $(0,\infty)$, there are l values of τ, $\{\tau_i\}_{i=1}^{l} \subset (0,\infty)$ where a negative eigenvalue of $\mathscr{U}^*.\mathscr{M}_\tau\mathscr{U}$ crosses 0 and

$$\begin{aligned}\ell &= \mathbb{D}^-[\mathscr{U}^*.\mathscr{M}_0\mathscr{U}] - \mathbb{D}^-[\mathscr{U}^*.\mathscr{M}_T\mathscr{U}] = \mathbb{D}^-[.\mathscr{M}_0] - \mathbb{D}^-[.\mathscr{M}_T] \\ &= \mathbb{D}^-[.\mathscr{A} - \eta.\mathscr{B}] - (\operatorname{null}[\mathscr{C}] + \mathbb{D}^-[\mathscr{C}]) + \dim(\operatorname{Ker}(.\mathscr{A}) \cap \operatorname{Ker}(.\mathscr{B}))\ .\end{aligned}$$

Thus for each $i = 1, 2, \ldots, l$, $\eta - \tau_i$ is a discrete eigenvalue of $.\mathscr{A}\mathbf{x} = \zeta.\mathscr{B}\mathbf{x}$ in $(-\infty, \eta)$. Conversely, every discrete eigenvalue of $.\mathscr{A}\mathbf{x} = \zeta.\mathscr{B}\mathbf{x}$ in $(-\infty, \eta)$ must occur at such a zero crossing and so must equal $\eta - \tau_i$ for some $i = 1, \ldots, l$.

Now, observe that $p - \nu(\eta)$ is the number of discrete eigenvalues of $.\mathscr{A}\mathbf{x} = \zeta.\mathscr{B}\mathbf{x}$ in the open interval $(-\infty, \eta)$. Thus $p - \nu(\eta) = l$. Recall from Definition (3.1), $\operatorname{null}[.\mathscr{A} - \eta.\mathscr{B}] = \nu(\eta) + \dim[\operatorname{Ker}(.\mathscr{A}) \cap \operatorname{Ker}(.\mathscr{B})]$, hence (3.5) is established. □

This leads us to our main result.

Theorem 3.3. *Let μ and r be chosen so that $\mu \leq \lambda_r^0$. Suppose that $\{p_i\}_{i=1}^{k} \subset \operatorname{Dom}(T^*)$ and $\{q_i\}_{i=1}^{n} \subset \operatorname{Dom}(A_0)$. If the generalized matrix eigenvalue problem*

$$\begin{bmatrix} .\mathscr{F}_1 & 0 \\ 0 & .\mathscr{F}_2 \end{bmatrix} \begin{Bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{Bmatrix} = \zeta \begin{bmatrix} .\mathscr{G}_1 & .\mathscr{H} \\ .\mathscr{H}^* & .\mathscr{G}_2 \end{bmatrix} \begin{Bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{Bmatrix}$$

has discrete finite eigenvalues ordered as

$$\zeta_1 \leq \zeta_2 \leq \ldots \leq \zeta_\ell < 0 \leq \zeta_{\ell+1} \ldots$$

($\ell = 0$ if all discrete eigenvalues are either nonnegative or infinite), then $\ell = \mathbb{D}^-[.\mathscr{F}_1] - d$, where $d = \operatorname{null}[\mathscr{C}] + \mathbb{D}^-[\mathscr{C}] - (\operatorname{null}[.\mathscr{G}_1] + \operatorname{null}[.\mathscr{F}_2])$ for $\mathscr{C} = \mathscr{V}^*.\mathscr{F}_1\mathscr{V}_1 + \mathscr{V}_2^*.\mathscr{F}_2\mathscr{V}_2$ with $\mathscr{V} = \begin{bmatrix} \mathscr{V}_1 \\ \mathscr{V}_2 \end{bmatrix}$ having columns that form a basis for $\operatorname{Ker}\left(\begin{bmatrix} .\mathscr{G}_1 & .\mathscr{H} \\ .\mathscr{H}^* & .\mathscr{G}_2 \end{bmatrix}\right)$. Furthermore, for each eigenvalue ζ_p with $p \leq \ell$ we have a corresponding lower bound for an eigenvalue of A,

$$\mu + \frac{1}{\zeta_p} \leq \lambda_{r-d-m(p)} \leq \lambda_{r-d-p} \leq \lambda_{r-p}$$

where $m(p) = \max\{m | \zeta_m = \zeta_p\}$.

Proof. In Lemma 3.2, consider $.\mathscr{A} = \begin{bmatrix} .\mathscr{F}_1 & 0 \\ 0 & .\mathscr{F}_2 \end{bmatrix}$, $.\mathscr{B} = \begin{bmatrix} .\mathscr{G}_1 & .\mathscr{H} \\ .\mathscr{H}^* & .\mathscr{G}_2 \end{bmatrix}$, and $\mathscr{C}$ as given above. Setting $\eta = 0$ in (3.5) and observing that $\dim(\operatorname{Ker}(.\mathscr{A}) \cap \operatorname{Ker}(.\mathscr{B})) = \operatorname{null}(.\mathscr{G}_1) + \operatorname{null}(.\mathscr{F}_2)$, we find

$$\begin{aligned}\ell &= \operatorname{null}[\mathscr{A}] + \mathbb{D}^-[\mathscr{A}] - (\operatorname{null}(\mathscr{C}) + \mathbb{D}^-[\mathscr{C}]) - \nu(0)\\ &= (\nu(0) + \dim(\operatorname{Ker}(\mathscr{A}) \cap \operatorname{Ker}(\mathscr{B})) + \mathbb{D}^-[\mathscr{F}_1] - (\operatorname{null}(\mathscr{C}) + \mathbb{D}^-[\mathscr{C}]) - \nu(0)\\ &= \mathbb{D}^-[\mathscr{F}_1] - (\operatorname{null}(\mathscr{C}) - \dim(\operatorname{Ker}(\mathscr{A}) \cap \operatorname{Ker}(\mathscr{B})) + \mathbb{D}^-[\mathscr{C}])\\ &= \mathbb{D}^-[\mathscr{F}_1] - d\ .\end{aligned}$$

The last two inequalities of (3.6) follow trivially from the easily verified assertions, $d \geq 0$ and $p \leq m(p)$. To show the remaining inequality, in the hypothesis of Lemma 3.2, set $\eta = \zeta_p = \zeta_m(p)$ for some $p \leq \ell$. Then from (3.3) and the observation that $N_0(\mu) \leq r - 1$, we have for every $\lambda \leq \mu + \frac{1}{\zeta_p}$,

$$\begin{aligned}N(\lambda) &\leq N_0(\mu) - \{m(p) + \operatorname{null}[\mathscr{C}] + \mathbb{D}^-(\mathscr{C})\} + \operatorname{null}(\mathscr{G}_1) + \operatorname{null}(\mathscr{F}_2)\\ &\leq (r-1) - m(p) - d\ .\end{aligned}$$

Thus, every such λ is a lower bound to $\lambda_{r-d-m(p)}$. □

The index parameter "*d*" provides a correction to *a priori* information available for A_0 (given in the form of the index "*r*"). This correction is based (perhaps somewhat mysteriously) in part on computable information about $\operatorname{Ker}\left(\begin{bmatrix}\mathscr{G}_1 & \mathscr{H}\\ \mathscr{H}^* & \mathscr{G}_2\end{bmatrix}\right)$. In order to better understand the source of this correction, let us now assume that $\{(A_0-\mu)q_i\}_{i=1}^n$ and $\{T^*p_i\}_{i=1}^k$ are separately linearly independent sets but $\mathfrak{M} = \operatorname*{span}_{i=1,\ldots,n}(A_0-\mu)q_i \cap \operatorname*{span}_{i=1,\ldots,k} T^*p_i$ is non-trivial. This implies that $\mathscr{G}_1$, $\mathscr{G}_2$, and $\mathscr{F}_2$ are nonsingular but $\begin{bmatrix}\mathscr{G}_1 & \mathscr{H}\\ \mathscr{H}^* & \mathscr{G}_2\end{bmatrix}$ is singular. Let $\nu = \dim\mathfrak{M} = \operatorname{null}\left(\begin{bmatrix}\mathscr{G}_1 & \mathscr{H}\\ \mathscr{H}^* & \mathscr{G}_2\end{bmatrix}\right)$ and $\tau = n - \nu$. There exist matrices $\mathscr{V}_1 = [v_{ij}^{(1)}] \in \mathbb{C}^{n\times\nu}$ and $\mathscr{V}_2 = [v_{ij}^{(2)}] \in \mathbb{C}^{k\times\nu}$ such that $\operatorname{rank}[\mathscr{V}_1] = \operatorname{rank}[\mathscr{V}_2] = \nu$ and

$$\begin{bmatrix}\mathscr{G}_1 & \mathscr{H}\\ \mathscr{H}^* & \mathscr{G}_2\end{bmatrix}\begin{bmatrix}\mathscr{V}_1\\ \mathscr{V}_2\end{bmatrix} = \mathbf{0}\ .$$

Define $\tilde{q}_j = \sum_{i=1}^n v_{ij}^{(1)} q_i$ and $\tilde{p}_j = \sum_{i=1}^k v_{ij}^{(2)} p_i$ for $j = 1, 2, \ldots, \nu$. For convenience, we will assume that μ is in the resolvent set for A_0, although this ultimately entails no loss of generality. Then $(A_0-\mu)\tilde{q}_j + T^*\tilde{p}_j = 0$ and we may compute

$$\begin{aligned}\mathscr{C} &= [\mathscr{V}_1^*\mathscr{V}_2^*]\begin{bmatrix}\mathscr{F}_1 & 0\\ 0 & \mathscr{F}_2\end{bmatrix}\begin{bmatrix}\mathscr{V}_1\\ \mathscr{V}_2\end{bmatrix} = \mathscr{V}_2^*\mathscr{F}_2\mathscr{V}_2 + \mathscr{V}_1\mathscr{F}_1\mathscr{V}_1\\ &= [\langle\tilde{p}_i, \tilde{p}_j\rangle_* + \langle\tilde{q}_i, (A_0-\mu)\tilde{q}_j\rangle]\\ &= [\langle\tilde{p}_i, \tilde{p}_j\rangle_* + \langle R_\mu^0 T^*\tilde{p}_i, T^*\tilde{p}_j\rangle] = \mathscr{W}_\nu(\mu)\ ,\end{aligned}$$

which is the W-A matrix for an intermediate problem that we may write as $A_\nu = A_0 + T^*\tilde{P}_\nu T$. Notice now from (2.4), $N_\nu(\mu) = N_0(\mu) - \{\operatorname{null}[\mathscr{W}_\nu(\mu)] + \mathbb{D}^-[\mathscr{W}_\nu(\mu)]\} = r - d$.

Thus, computable information about $\operatorname{Ker}\begin{bmatrix}\mathscr{G}_1 & \mathscr{H}\\ \mathscr{H}^* & \mathscr{G}_2\end{bmatrix}$ is used to determine where μ lies in the spectrum of the intermediate operator A_ν. Since A_ν dominates

A_0 in the sense of quadratic forms, this provides in a certain sense stronger *a priori* information than was initially available from just A_0.

3.3. The EVF method

For clarity we lay out a methodology that Theorem 3.3 suggests for computing lower bounds to the eigenvalues of A. For compactness, we refer to the following as the EVF (**E**igen**v**ector **F**ree method):

(1) Select trial vectors $\{q_i\}_{i=1}^n \subset \mathrm{Dom}(A_0)$ and $\{p_j\}_{j=1}^k \subset \mathrm{Dom}(T^*)$.
(2) Pick (or compute) a value $\mu \in (\lambda_{r-1}^0, \lambda_r^0]$ for a selected $r > 1$.
(3) Form and solve the matrix eigenvalue problem defined by (3.4).
(4) The finite negative discrete eigenvalues computed from (3.4) may each be associated with eigenvalue bounds as given in (3.6).

Although we need only assume $\mu \leq \lambda_r^0$ in order to deduce the bounds given in (3.6), one should seek to choose μ and r so that $\mu \in (\lambda_{r-1}^0, \lambda_r^0]$. Otherwise, $N_0(\mu) \leq r - 1$ and it will be infeasible to have lower bounds convergent to the correspondingly indexed eigenvalues of A (see also [9] and [10]).

Notice that if both A_0 and T^* are local operators and the vectors $\{q_i\}_{i=1}^n$ and $\{p_j\}_{j=1}^k$ are chosen to have local support (as with, for example, finite-element trial functions), then the resulting matrices will be sparse and (3.4) may be efficiently handled using sparse matrix techniques, even for quite large values of n and k. Furthermore, the only need for *a priori* spectral information comes through the selection (or computation) of μ as a sufficiently good lower bound to λ_r^0 to separate it from λ_{r-1}^0. No eigenvector data for A_0 are necessary nor are "exact" values for the eigenvalues of A_0 needed for appropriate selection of μ.

3.4. Using $B = T^*T$ directly

In some circumstances, it may be more convenient to consider the use of the operator $B = T^*T$ and avoid the use of T^* altogether. An alternate development using B is quite straightforward and proceeds in direct analogy with what has gone before. We provide only an outline here. Pick projecting vectors $\{p_1, p_2, \ldots\} \subset \mathrm{Dom}(B)$ instead and define the B-orthogonal projection onto $\underset{i=1,\ldots,k}{\mathrm{span}}\ \{p_i\}$

$$P_k u = \sum_{i,j=1}^{k} \langle u, Bp_i \rangle . \mathscr{B}_{ij} p_i$$

where $[.\mathscr{B}_{ij}]$ is the Moore–Penrose generalized inverse to $[\langle Bp_i, p_i \rangle]$. Now define $B_k = BP_k + \delta^2 I$. The operator B_k is bounded, self-adjoint, positive-definite, and has an explicit inverse given by

$$B_k^{-1}v = \frac{1}{\delta^2}\left[v - \sum_{l,m=1}^{k} \langle v, Bp_l\rangle \mathscr{C}_{lm} Bp_m\right]$$

where $[\mathscr{C}_{lm}]$ is the Moore–Penrose generalized matrix inverse to $[\delta^2\langle Bp_i, p_j\rangle + \langle Bp_i, Bp_j\rangle]$ (instead of (2.8)). Likewise (3.1) becomes

$$\mathscr{W}_{k,n}(\lambda) = [\langle q_i, (A_0-\mu)q_i\rangle] + \frac{1}{\mu-\lambda}\Big\{\langle (A_0-\mu)q_i, (A_0-\mu)q_j\rangle - \sum_{l,m=1}^{k}\langle (A_0-\mu)q_i, Bp_l\rangle \mathscr{C}_{lm}\langle Bp_m, (A_0-\mu)q_j\rangle\Big\}$$

Proceeding in a like manner, we arrive finally to the analog of Theorem 3.3 which we state without proof.

Theorem 3.4. *Let μ and r be chosen so that $\mu \le \lambda_r^0$. Suppose that $\{p_i\}_{i=1}^k \subset \mathrm{Dom}(B)$ and $\{q_i\}_{i=1}^n \subset \mathrm{Dom}(A_0)$.*

Define the following matrices

$$\begin{aligned}
\mathscr{F}_1 &= [\langle q_i, (A_0-\mu)q_i\rangle] \in \mathbb{C}^{n\times n}\\
\mathscr{G}_1 &= [\langle (A_0-\mu)q_i, (A_0-\mu)q_j\rangle] \in \mathbb{C}^{n\times n}\ ,\\
\mathscr{F}_2 &= [\langle p_i, Bp_j\rangle] \in \mathbb{C}^{k\times k}\ ,\\
\mathscr{G}_2 &= [\langle Bp_i, Bp_j\rangle] \in \mathbb{C}^{k\times k}\ ,
\end{aligned}$$

and

$$\mathscr{H}[\langle (A_0-\mu)q_i, Bp_j\rangle] \in \mathbb{C}^{n\times k}\ .$$

If the generalized matrix eigenvalue problem

$$\begin{bmatrix}\mathscr{F}_1 & 0\\ 0 & \mathscr{F}_2\end{bmatrix}\begin{Bmatrix}x_1\\ x_2\end{Bmatrix} = \zeta\begin{bmatrix}\mathscr{G}_1 & \mathscr{H}\\ \mathscr{H}^* & \mathscr{G}_2\end{bmatrix}\begin{Bmatrix}x_1\\ x_2\end{Bmatrix}$$

has discrete finite eigenvalues ordered as

$$\zeta_1 \le \zeta_2 \le \ldots \zeta_\ell < 0 \le \zeta_{\ell+1} \le \ldots$$

($\ell = 0$ if all discrete eigenvalues are either nonnegative or infinite), then for each eigenvalue ζ_p with $p \le \ell$ we have a correspronding lower bound for an eigenvalue of A

$$\mu + \frac{1}{\zeta_p} \le \lambda_{r-d-m(p)} \le \lambda_{r-d-p} \le \lambda_{r-p}$$

where $m(p) = \max\{m\,|\,\xi_m = \xi_p\}$ and $d = \mathrm{null}[\mathscr{C}] + \mathbb{D}^-[\mathscr{C}] - \mathrm{null}[\mathscr{G}_1] + \mathrm{null}[\mathscr{F}_2]$) for $\mathscr{C} = \mathscr{V}_1^*\mathscr{F}_1\mathscr{V}_1 + \mathscr{V}_2^*\mathscr{F}_2\mathscr{V}_2$ with $\mathscr{V} = \begin{bmatrix}\mathscr{V}_1\\ \mathscr{V}_2\end{bmatrix}$ having columns that form a basis for $\mathrm{Ker}\left(\begin{bmatrix}\mathscr{G}_1 & \mathscr{H}\\ \mathscr{H}^* & \mathscr{G}_2\end{bmatrix}\right)$.

4. Parameter selection

4.1. Monotonicity of bounds with respect to μ

Typically one will have a range of feasible μ values available within the interval we discover here is that the best in the interval $(\lambda_{r-1}^0, \lambda_r^0]$. What we discover here is that the best available lower bound to λ_r^0 in the interval $(\lambda_{r-1}^0, \lambda_r^0]$ produces the best bound in (3.6).

Theorem 4.1. *The lower bound $\mu + \frac{1}{\zeta_p(\mu)}$ in (3.6) is monotone increasing in μ on $(\lambda_{r-1}^0, \lambda_r^0]$.*

Proof. Fix a nonzero vector $\mathbf{x} \in \mathbb{C}^n$, define $\hat{q} = \sum_{i=1}^n x_i q_i$, and introduce the function $\Phi(\mu, \lambda) = \mathbf{x}^* \mathscr{W}_{k,n}(\mu, \lambda)\mathbf{x}$ where $\mathscr{W}_{k,n}(\mu, \lambda)$, defined by (3.1), now shows explicitly the dependence on μ. Φ is continuously differentiable for $\lambda < \mu$ and we have

$$\frac{\partial \Phi}{\partial \mu} = \langle (A_0 - \mu)\hat{q}, \left[\frac{\partial B_k^{-1}}{\partial \mu}\right](A_0 - \mu)\hat{q}\rangle - \langle \hat{q}, B_k^{-1}(A_0 - \mu)\hat{q}\rangle - \langle (A_0 - \mu)\hat{q}, B_k^{-1}\hat{q}\rangle - \|\hat{q}\|^2 .$$

From the definition of B_k, $\frac{\partial B_k^{-1}}{\partial \mu} = -B_k^{-1}\left[\frac{\partial B_k}{\partial \mu}\right]B_k^{-1} = B_k^{-2}$, hence

$$\frac{\partial \Phi}{\partial \mu} = -\|B_k^{-1}(A_0 - \mu)\hat{q} + \hat{q}\|^2 \leq 0 .$$

Likewise,

$$\frac{\partial \Phi}{\partial \lambda} = \langle (A_0 - \mu)\hat{q}, \left[\frac{\partial B_k^{-1}}{\partial \lambda}\right](A_0 - \mu)\hat{q}\rangle = \|B_k^{-1}(A_0 - \mu)\hat{q}\|^2 \geq 0 .$$

This establishes that Φ is monotone decreasing in μ and monotone increasing in λ over the range of values $\lambda < \mu$. Thus, for $\lambda_1 < \lambda_2 < \mu_1 < \mu_2$ we have

$$\mathscr{W}_{k,n}(\mu, \lambda_1) \leq \mathscr{W}_{k,n}(\mu, \lambda_2) \quad \text{for} \quad \lambda_1 < \lambda_2 < \mu \tag{4.1}$$

and

$$\mathscr{W}_{k,n}(\mu_1, \lambda) \leq \mathscr{W}_{k,n}(\mu_2, \lambda) \quad \text{for} \quad \lambda < \mu_1 < \mu_2 . \tag{4.2}$$

For compactness, we now fix the indices k, n and suppress them in our notation. Define for each $0 \leq J < r$ and $\mu \in (\lambda_{r-1}^0, \lambda_r^0]$,

$$\Gamma_J(\mu) = \{\lambda | \text{null}\,[\mathscr{W}(\mu, \lambda)] + \mathbb{D}^-[\mathscr{W}(\mu, \lambda)] \leq r - J\} .$$

Then $\lambda \in \Gamma_J(\lambda)$ implies that $\lambda \leq \lambda_{J+1}$ from (3.3). From (4.1), $\text{null}\,[\mathscr{W}(\mu, \lambda)] + \mathbb{D}^-[\mathscr{W}(\mu, \lambda)]$ is increasing as λ decreases, hence if $\lambda \in \Gamma_J(\mu)$ then $(-\infty, \lambda] \subset \Gamma_J(\mu)$ as well. For $1 \leq p < \ell$ and $J = r - m(p) - 1$ we have

$$\mu + \frac{1}{\zeta_p} \in \Gamma_J(\mu) \ .$$

Furthermore $\mu + \frac{1}{\zeta_p} = \max\{\Gamma_J(\mu)\}$. To see this, define $\lambda(\epsilon) = \mu + (\zeta_p - \epsilon)^{-1}$ for $\epsilon > 0$ and $\lambda(0) = \mu + \frac{1}{\zeta_p}$. Then evidently $\lambda(0) < \lambda(\epsilon)$ and

$$\begin{aligned}\text{null}\,[\mathscr{W}(\mu,\lambda(\epsilon))] + \mathbb{D}^-[\mathscr{W}(\mu,\lambda(\epsilon))] &= \text{null}\,[\mathscr{M}(\zeta_p - \epsilon)] + \mathbb{D}^-[\mathscr{M}(\zeta_p - \epsilon)] \\ &< \text{null}\,[\mathscr{M}(\zeta_p)] + \mathbb{D}^-[\mathscr{M}(\zeta_p)] \\ &= \text{null}\,[\mathscr{W}(\mu,\lambda(0))] + \mathbb{D}^-[\mathscr{W}(\mu,\lambda(0))] = r - J \ .\end{aligned}$$

So $\lambda(\epsilon) \notin \Gamma_J(\mu)$ for any $c > 0$. The proof is completed by observing from (4.2) that for $\mu_1 < \mu_2$, $\Gamma_J(\mu_1) \subset \Gamma_J(\mu_2)$. Thus,

$$\mu_1 + \frac{1}{\zeta_p(\mu_1)} = \max\{\Gamma_J(\mu_1\} \le \max\{\Gamma_J(\mu_2)\} = \mu_2 + \frac{1}{\zeta_p(\mu_2)} \ . \qquad \square$$

4.2. Monotonicity with respect to dimension

For fixed μ it is natural to expect the bounds provided by (3.4)–(3.6) to improve as the dimensions of the approximating subspaces increase. We state this formally as

Theorem 4.2. *Let* $\{q_i\}_{i=1}^N \subset \text{Dom}\,(A_0)$ *and* $\{p_j\}_{j=1}^K \subset \text{Dom}\,(T^*)$ *be fixed sets of vectors. For* $1 \le \nu \le N$, $1 \le \kappa \le K$, *and fixed* μ, *let* $\zeta_p^{(\nu,\kappa)}$ *be the* p*th negative discrete eigenvalue of (3.4) corresponding to the use of* $\{q_i\}_{i=1}^\nu$ *and* $\{p_j\}_{j=1}^\kappa$. *If* $1 \le \nu_1 \le \nu_2 \le N$ *and* $1 \le \kappa_1 \le \kappa_2 \le K$ *then*

$$\mu + \frac{1}{\zeta_p^{(\nu_1,\kappa_1)}} \le \mu + \frac{1}{\zeta_p^{(\nu_2,\kappa_2)}} \le \lambda_{r-p} \ .$$

Proof. In view of (3.5), it is sufficient to show $\zeta_p^{(\nu_2,\kappa_2)} \le \zeta_p^{(\nu_1,\kappa_1)}$, or equivalently that for each ν, κ satisfying $1 \le \nu \le N-1$ and $1 \le \kappa \le K$ we have $\zeta_p^{(\nu+1,\kappa)} \le \zeta_p^{(\nu,\kappa)}$, and for each ν, κ satisfying $1 \le \nu \le N$ and $1 \le \kappa \le K$ we have $\zeta_p^{(\nu,\kappa+1)} \le \zeta_p^{(\nu,\kappa)}$. In either case, the Cauchy interlace theorem [cf. 31] provides the conclusion. $\square$

5. Relationship with other methods

5.1. Truncated intermediate problems

The derivation in Sect. 3.1 clearly indicates the close association the EVF method has with the standard method of intermediate problems. To emphasize this, we show how to recover the method of truncation [3] by an appropriate choice of

trial vectors in the EVF method. If we select $q_i = u_i^0$ for $i = 1, \ldots, n$ and suppose $\mu = \lambda_{n+1}^0 > \lambda_n^0$, the matrix eigenvalue problem (3.4) reduces to a diagonal scaling of the matrix eigenvalue problem used for the method of truncation applied with the same projecting vectors $\{p_i\}_{i=1}^k$. In particular, set $\hat{\mathscr{R}} = [\langle T^* p_i, T^* p_j \rangle]$, $\hat{\mathscr{S}} = [\langle T^* p_i, u_\nu^0 \rangle]$, $\hat{\mathscr{T}} = [\langle p_i, p_j \rangle_*]$, and $\Lambda = \operatorname{diag}_{i=1,\ldots,n} (\lambda_i^0)$. Then explicitly

$$\begin{bmatrix} I & \hat{\mathscr{S}} \\ \hat{\mathscr{S}}^* & \hat{\mathscr{R}} \end{bmatrix} - (\lambda - \mu) \begin{bmatrix} (\Lambda - \mu I)^{-1} & 0 \\ 0 & \hat{\mathscr{T}} \end{bmatrix}$$
$$= -\mathscr{D} \left(\begin{bmatrix} \mathscr{T}_1 & 0 \\ 0 & \mathscr{T}_2 \end{bmatrix} - \zeta \begin{bmatrix} \mathscr{G}_1 & \mathscr{H} \\ \mathscr{H}^* & \mathscr{G}_2 \end{bmatrix} \right) \mathscr{D}$$

where $\mathscr{D} = \sqrt{\mu - \lambda} \begin{bmatrix} (\Lambda - \mu)^{-1} & 0 \\ 0 & I \end{bmatrix}$.

The left-hand matrix pencil matches equation (5) of [8] giving computable conditions on λ to be an eigenvalue of the truncated intermediate operator below the truncation point μ.

5.2. Temple-Lehmann-Maehly methods

One may observe also a close connection with methods that are associated with Temple, Lehmann, and Maehly. If we take $A_0 = A$ (so that $T = 0$), then μ becomes a separating parameter for λ_{r-1} and λ_r and the eigenvalue problem (3.4) reduces to $\mathscr{T}_1 \mathbf{x} = \zeta \mathscr{G}_1 \mathbf{x}$ or explicitly,

$$[\langle q_i, (A - \mu) q_j \rangle] \mathbf{x} = \zeta [\langle (A - \mu) q_i, (A - \mu) q_j \rangle] \mathbf{x} \,. \tag{5.1}$$

The bounds given in (3.6) ($d = 0$ in this case) conform to those originally given by Lehmann in [26] and [27] and by Maehly in [28]. In the scalar case ($n = 1$) we recover from (3.6) Temple's inequality

$$\mu + \frac{\|(A - \mu) q\|^2}{\langle q, (A - \mu) q \rangle} \leq \lambda_{r-1} \,. \tag{5.2}$$

The Temple-Lehmann-Maehly methods may be directly linked to the method of intermediate problems via the analysis of Sects. 3.1–3.2. In fact, the Lehmann-Maehly eigenvalue problem (5.1) arises spontaneously from the Weinstein-Aronszajn matrix corresponding to the parameterized intermediate problem

$$A_n^\theta = A - \theta + \theta P_n$$

where P_n is an orthogonal projection onto $\operatorname{span}_{i=1,\ldots,n} \{(A - \mu) q_i\}$ and the parameter values θ satisfy the side constraint, $\lambda + \theta = \mu$.

A broader relationship with the "Temple quotient" appearing on the left-hand side of (5.2) may be observed by expressing the bound $\mu + \frac{1}{\zeta_p}$ in terms

of the Rayleigh quotient for the matrix eigenvalue, ζ_p. Suppose $\left\{ \begin{matrix} \mathbf{x} \\ \mathbf{y} \end{matrix} \right\}$ is an eigenvector of the matrix pencil (3.4) associated with the eigenvalue ζ_p, and let $\{x_i\}\{y_i\}$ denote the components of $\mathbf{x}$ and $\mathbf{y}$, respectively. If $q = \sum_{i=1}^{n} x_i q_i$ and $p = \sum_{i=1}^{k} y_i p_i$ then

$$\mu + \frac{1}{\zeta_p} = \mu + \frac{\|(A_0 - \mu)q + T^* p\|^2}{\langle q, (A_0 - \mu)q\rangle + \|p\|_*^2}$$

Notice that if $p = T_q$ (which presupposes that $\mathrm{Dom}\,(A_0) \cap \mathrm{Dom}\,(T^*T)$ is nontrivial) then the right-hand side reduces to the Temple quotient in (5.2).

5.3. Weinberger's method

In 1959, Weinberger [34] introduced a method for computing eigenvalue lower bounds that was substantially different from either of the previously known methods of Lehmann and Maehly or of Weinstein and Aronszajn, while in some measure generalizing them both. A key departure was the form of *a priori* spectral information taken for A. Following Weinberger [35, Sect. 4.9], we will assume for the moment that a finite dimensional space $\mathfrak{P}$ is explicitly known together with a parameter μ such that

$$\langle Av, v\rangle \geq \mu \|v\|^2 \quad \text{for all} \quad v \in \mathfrak{P}^{\perp} \tag{5.3}$$

If $\dim \mathfrak{P} = k$, note that (5.3) implies that $\mu \leq \lambda_{k+1}$. Weinberger's method proceeds by selecting a basis for $\mathfrak{P}$, $\{p_1, p_2, \ldots, p_k\}$, and a set of trial vectors, $\{q_1, q_2, \ldots, q_n\} \subset \mathrm{Dom}\,(A)$, and considering the generalized matrix eigenvalue problem

$$\begin{bmatrix} \mathscr{R} & \mathscr{S}_1 \\ \mathscr{S}_1{}^* & 0 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} = \zeta \begin{bmatrix} \mathscr{T}_1 & \mathscr{S}_2 \\ \mathscr{S}_2{}^* & \mathscr{T}_2 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} \tag{5.4}$$

$$\begin{aligned} \text{where} \quad \mathscr{R} &= [\langle q_i, (A - \mu)q_j\rangle] \in \mathbb{C}^{n\times n}\,, \\ \mathscr{S}_1 &= [\langle q_i, p_j\rangle] \in \mathbb{C}^{n\times k}\,, \\ \mathscr{S}_2 &= [\langle (A - \mu)q_i, p_j\rangle] \in \mathbb{C}^{n\times k}\,, \\ \mathscr{T}_1 &= [\langle (A - \mu)q_i, (A - \mu)q_j\rangle] \in \mathbb{C}^{n\times n} \\ \text{and} \quad \mathscr{T}_2 &= [\langle p_i, p_j\rangle] \in \mathbb{C}^{k\times k}\,. \end{aligned}$$

Eigenvalue bounds may be deduced as a consequence of the following theorem. This theorem is essentially similar to one originally given by Weinberger (Chapter 4, Theorem 9.3 of [35]), however $\mathrm{null}\,(\mathscr{C}) = 0$ replaces Weinberger's original hypothesis: $\mathrm{rank}\left(\begin{bmatrix} \mathscr{R} & \mathscr{S}_1 \\ \mathscr{S}_1{}^* & 0 \end{bmatrix}\right) = \rho + n$. See the discussion below.

Theorem 5.1. *Let $\mathfrak{P}$ and μ be known so that (5.3) holds. Define $r = 1 + k = 1 + \dim \mathfrak{P}$ and $\rho = \mathrm{rank}\,(\mathscr{S}_1)$. Let $\mathscr{V}$ have columns that* $\mathrm{span}\,\mathrm{Ker}\left(\begin{bmatrix} \mathscr{T}_1 & \mathscr{S}_2 \\ \mathscr{S}_2{}^* & \mathscr{T}_2 \end{bmatrix}\right)$,

and suppose that $\mathscr{C} = \mathscr{V}^* \begin{bmatrix} \mathscr{R} & \mathscr{S}_1 \\ \mathscr{S}_1^* & 0 \end{bmatrix} \mathscr{V}$ *is nonsingular. If the finite discrete eigenvalues of (5.4) are ordered as*

$$\zeta_1 \leq \zeta_2 \leq \ldots \leq \zeta_l < 0 \leq \zeta_{l+1} \ldots$$

($l = 0$) *if all discrete eigenvalues are either nonnegative or infinite) then for each eigenvalue* ζ_p *with* $p \leq l$ *we have a corresponding lower bound for an eigenvalue of A,*

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

where $\delta = \rho - l$.

Proof. Let P denote an orthogonal projection onto $\mathfrak{P}$. For $\epsilon > 0$, define $A_0(\epsilon) = A - \frac{1}{\epsilon}P$. We first assert that $\mu \leq \lambda_r^0(\epsilon)$ for any $\epsilon > 0$. If this were not the case then there would be an r-dimensional subspace $\mathfrak{U}_\epsilon$ such that $\langle u, A_0(\epsilon)u\rangle < \mu\|u\|^2$ for all $u \in \mathfrak{U}_\epsilon$. But since $\dim \mathfrak{U}_\epsilon > \dim \mathfrak{P}$, there exists a nontrivial $\bar{u} \in \mathfrak{U}_\epsilon \cap \mathfrak{P}^\perp$ and (5.3) implies $\langle \bar{u}, A_0(\epsilon)\bar{u}\rangle = \langle \bar{u}, A\bar{u}\rangle \geq \mu\|\bar{u}\|^2$ which produces a contradiction. Thus $\mu \leq \lambda_r^0(\epsilon)$, as asserted.

We define $T(\epsilon) = \frac{1}{\sqrt{\epsilon}}P$ and apply Theorem 3.3 with the decomposition $A = A_0(\epsilon) + T^*(\epsilon)T(\epsilon)$:

$$\mathscr{T}_1(\epsilon) = \mathscr{R} - \frac{1}{\epsilon}\mathscr{S}_1\mathscr{T}_2^{-1}\mathscr{S}_1^*$$

$$\mathscr{T}_2 = \mathscr{T}_2$$

$$\mathscr{G}_1(\epsilon) = \mathscr{T}_1 - \frac{1}{\epsilon}\mathscr{S}_1\mathscr{T}_2^{-1}\mathscr{S}_2^* - \frac{1}{\epsilon}\mathscr{S}_2\mathscr{T}_2^{-1}\mathscr{S}_1^* + \frac{1}{\epsilon^2}\mathscr{S}_1\mathscr{T}_2^{-1}\mathscr{S}_1^*$$

$$\mathscr{G}_2(\epsilon) = \frac{1}{\epsilon}\mathscr{T}_2$$

$$\text{and } \mathscr{H}(\epsilon) = \frac{1}{\sqrt{\epsilon}}\left[\mathscr{S}_1 - \frac{1}{\epsilon}\mathscr{S}_2\right].$$

$$\text{Define } X_\epsilon = \begin{bmatrix} I & \frac{1}{\sqrt{\epsilon}}\mathscr{S}_1\mathscr{T}_2^{-1} \\ 0 & \sqrt{\epsilon}I \end{bmatrix} \quad \text{and observe}$$

$$\text{(5.5)} \qquad \begin{aligned} X_\epsilon \left(\begin{bmatrix} \mathscr{T}_1(\epsilon) & 0 \\ 0 & \mathscr{T}_2 \end{bmatrix} - \zeta \begin{bmatrix} \mathscr{G}_1(\epsilon) & \mathscr{H}(\epsilon) \\ \mathscr{H}^*(\epsilon) & \mathscr{G}_2(\epsilon) \end{bmatrix} \right) X_\epsilon^* \\ = \begin{bmatrix} \mathscr{R} & \mathscr{S}_1 \\ \mathscr{S}_1^* & \epsilon\mathscr{T}_2 \end{bmatrix} - \zeta \begin{bmatrix} \mathscr{T}_1 & \mathscr{S}_2 \\ \mathscr{S}_2^* & \mathscr{T}_2 \end{bmatrix} \end{aligned}$$

Let $\mathscr{A}_\epsilon = \begin{bmatrix} \mathscr{R} & \mathscr{S}_1 \\ \mathscr{S}_1^* & \epsilon\mathscr{T}_2 \end{bmatrix}$, $\mathscr{A} = \begin{bmatrix} \mathscr{R} & \mathscr{S}_1 \\ \mathscr{S}_1^* & 0 \end{bmatrix}$, and $\mathscr{B} = \begin{bmatrix} \mathscr{T}_1 & \mathscr{S}_2 \\ \mathscr{S}_2^* & \mathscr{T}_2 \end{bmatrix}$. Define $\mathscr{C}_\epsilon = \mathscr{V}^*\mathscr{A}_\epsilon\mathscr{V}$ and notice that for all $\epsilon > 0$ sufficiently small, we have $\mathbb{D}^-[\mathscr{C}_\epsilon] = \mathbb{D}^-[\mathscr{C}]$ and null $[\mathscr{C}_\epsilon] = 0$. Furthermore, since null $[\mathscr{C}] = 0$ it is clear that Ker $\mathscr{A} \cap$ Ker $\mathscr{B} = \{0\}$. Thus, for any η not an eigenvalue of (5.4), $\mathbb{D}^-[\mathscr{A}_\epsilon - \eta\mathscr{B}] = \mathbb{D}^-[\mathscr{A} - \eta\mathscr{B}]$ for $\epsilon > 0$ sufficiently small. This implies for all such sufficiently

small $\epsilon > 0$, the matrix pencil (5.5) will have exactly $l = \mathbb{D}^-[\mathscr{A}] - \mathbb{D}^-[\mathscr{C}] = \mathbb{D}^-[\mathscr{A}_\epsilon] - \mathbb{D}^-[\mathscr{C}_\epsilon]$ negative eigenvalues,

$$\zeta_1(\epsilon) \le \zeta_2(\epsilon) \le \ldots \le \zeta_l(\epsilon) < 0$$

Furthermore, since $\mathbb{D}^-[\mathscr{A}_\epsilon - \eta\mathscr{B}] \le \mathbb{D}^-[\mathscr{A} - \eta\mathscr{B}]$ for any $\epsilon > 0$ and any η, it follows that $\zeta_i \le \zeta_i(\epsilon)$ and $\lim_{\epsilon \to 0} \zeta_i(\epsilon) = \zeta_i$ for each $i = 1, \ldots, l$.

Because $\mathscr{F}_1(\epsilon) = \mathscr{R} - \frac{1}{\epsilon}\mathscr{S}_1\mathscr{T}_2^{-1}\mathscr{S}_1^*$ and rank $(\mathscr{S}_1\mathscr{T}_2^{-1}\mathscr{S}_1^*)$ = rank $(\mathscr{S}_1) = \rho$, it is clear that $\mathbb{D}^-[\mathscr{F}_1(\epsilon)] \ge \rho$ for all $\epsilon > 0$ sufficiently small. Suppose $\mathbb{D}^-[\mathscr{F}_1(\epsilon)] > \rho$. Then there must be a nontrivial $\bar{q} \in \operatorname{span}_{i=1,\ldots,n} \{q_i\}$ such that $\langle \bar{q}_i, p_i \rangle = 0$ for $i = 1, \ldots, k$ and

$$0 > \langle \bar{q}, (A_0(\epsilon) - \mu)\bar{q} \rangle = \langle \bar{q}, (A - \frac{1}{\epsilon}P - \mu)\bar{q} \rangle = \langle \bar{q}, (A - \mu)\bar{q} \rangle \ ,$$

since $P\bar{q} = 0$. But this then contradicts (5.3) and we must have $\rho = \mathbb{D}^-[\mathscr{F}_1(\epsilon)]$ for all ϵ sufficiently small. Now Lemma 3.2 provides for all such ϵ, $\mathbb{D}^-[A_\epsilon] = \mathbb{D}^-[\mathscr{F}_1(\epsilon)] = \rho = l + d$. Thus $\delta = d$ and by Theorem 3.3

$$\mu + \frac{1}{\zeta_p(\epsilon)} \le \lambda_{r-d-p} = \lambda_{r-\delta-p} \quad \text{for} \quad p = 1, \ldots, l \ .$$

Since the bounds improve as ϵ is decreased further, taking $\epsilon \to 0$ yields the best bounds, and we arrive at the eigenvalue problem (5.4).

Although the assumption null $(\mathscr{C}) = 0$ is natural in the context of our Theorem 3.3, it is generally a stronger assumption than Weinberger's original: rank $\begin{bmatrix} \mathscr{R} & \mathscr{S}_1 \\ \mathscr{S}_1^* & 0 \end{bmatrix} = \rho + n$. In fact, if rank $\begin{bmatrix} \mathscr{R} & \mathscr{S}_1 \\ \mathscr{S}_1^* & 0 \end{bmatrix} < \rho + n$ then Ker $\begin{bmatrix} \mathscr{T}_1 & \mathscr{S}_2 \\ \mathscr{S}_2^* & \mathscr{T}_2 \end{bmatrix}$ is nontrivial and $\mathscr{C}$ is necessarily singular. The converse does not hold in general without additional hypotheses, such as null $\left(\begin{bmatrix} \mathscr{T}_1 & \mathscr{S}_2 \\ \mathscr{S}_2^* & \mathscr{T}_2 \end{bmatrix} \right) = k$.

6. Computational aspects

6.1. Some examples

We illustrate our method on two problems from technical mechanics. Return first to the consideration of the vibration of a fixed elastic solid begun in Sect. 2.

Example 1. (continued from Sect. 2.2). The Hilbert space $\mathfrak{H} = L^2(\Omega)^3$ can be decomposed into eight mutually orthogonal subspaces $\mathfrak{F}^{ijl}$ $(i, j, l \in \{0, 1\})$, each of which reduces the operator A (cf. [2]). Toward this end, define the following symmetry classes on $L_2(\Omega)$ for $i, j, l \in \{0, 1\}$,

$$\mathfrak{E}^{ijl}] = \{f \in L_2(\Omega) : f(x,y,z) = (-1)^i f(1-x,y,z) = (-1)^j f(x,1-y,z) = (-1)^l f(x,y,z,1-z)\}$$

Then for $i,j,l \in \{0,1\}$,

$$\mathfrak{F}^{ijl} = \left\{ \begin{pmatrix} f_1 \\ f_2 \\ f_3 \end{pmatrix} \in (L_2(\Omega))^3 : f_1 \in \mathfrak{E}^{v(i),j,l},\ f_2 \in \mathfrak{E}^{i,v(j),l},\ f_3 \in \mathfrak{E}^{i,j,v(l)} \right\},$$

$$\text{where } v(l) = \begin{cases} 1 & l = 0 \\ 0 & l = 1 \end{cases}.$$

Now let A^{ijl} be the restriction of A to $\mathfrak{F}^{ijl} \cap \mathrm{Dom}(A)$. Bounds to the eigenvalues of A can now be obtained by computing bounds to the eigenvalues of $A^{ijl}(i,j,l \in \{0,1\})$. Z. He [21] calculated bounds for A^{101} using trial functions built up from trigonometric functions. The bounds given in Table 1 and Table 2 are based on her results.

Table 1. Eigenvalue bounds for a linearly elastic cube

Eigenvalue index	A priori lower bounds	$\sigma = 1$		$\sigma = 100$	
		lower bounds	upper bounds	lower bounds	upper bounds
1	59.2176	60.6426	60.6430	62.1412	62.1421
2	59.2176	73.6596	73.6621	128.719	128.728
3	118.435	133.927	133.930	140.670	140.674
10	217.131	237.767	237.775	259.011	259.060
20	296.088	356.169	356.233	413.634	413.909
30	375.044	441.920	442.823	465.986	524.666

Lower bounds were computed with the EVF method of Sect. 3 for $n = 367$, $k = 64$, and $\mu = \lambda^0_{3,3,8} = 82\pi^2$. *A priori* lower bounds are obtained from the base problem. Upper bounds were computed with the Rayleigh-Ritz method with the same trial functions q_i used in the lower bound calculation.

Recall from [12] and the discussion at the end of Sect. 2.3 that the method of truncation provides eigenvalue bounds that are always at least good as those from the Bazley-Fox method of second projection. Since the method of second projection is central to our derivation, one might suspect that the method of truncation would also provide bounds that are at least as good as our method. This does not appear to be the general case. Table 2 provides bounds to the first eigenvalue of the Lamé operator ($\sigma = 100$) using both the method of truncation and the EVF method. For the method of truncation, $\tilde{n}$ denotes the truncation order and $\tilde{k}$ denotes the projecting subspace dimension. The same projecting subspaces were used in both methods. Notice that for higher order problems the EVF method provides slightly better bounds then does the method of truncation.

Example 2. The second example we consider arises in the modeling of the transverse free vibrations of a rotating beam which is clamped at the axis of rotation and free at the other end. This problem has been treated previously with other methods in [6] and [14]. The governing equation is

Table 2. Comparison of the Method of Truncation and the EVF method of Sect. 3.3

	Lower Bounds by Truncation		
$(\tilde{n}, \tilde{k})$	(24, 8)	(82, 64)	(196, 125)
	61.7852	62.0409	62.0975
	Lower Bounds by EVF		
(n, k)	(24, 8)	(81, 64)	(192, 125)
	61.7692	62.0815	62.1339

$$EI\frac{d^4u}{dx^4} - \frac{\rho\Omega^2}{2}\frac{d}{dx}(l^2 - x^2)\frac{du}{dx} = \omega^2\rho u$$

with boundary conditions $u(0) = u'(0) = 0 = u''(l) = u'''(l)$. Here, E is the modulus of elasticity, I is the moment of inertia of the cross section about the rotation axis, ρ is the lineal mass density, ρ is the angular velocity of rotation and l is the length of the beam.

After introducing the dimensionless variable $y = x/l$ we recast the problem as an operator eigenvalue problem on the Hilbert space $\mathfrak{H} = L_2(0, 1)$:

$$Au = \lambda u$$

where

$$A = \frac{d^4}{dy^4} - \frac{a^2}{2}\frac{d}{dy}(1 - y^2)\frac{d}{dy}$$

with $\mathrm{Dom}(A) = \{u \in H^4(0,1) | u(0) = u'(0) = u''(1) = u'''(1) = 0\}$, $\lambda = \omega^2\rho l^4/EI$, and $a^2 = \rho l^4\Omega^2/EI$.

The quadratic form associated with A is given by

$$a(u) = \int_0^1 \left(\left| \frac{d^2u}{dy^2} \right|^2 + \frac{a^2}{2}(1 - y^2) \left| \frac{du}{dy} \right|^2 \right) dy$$

with $\mathrm{Dom}(a) = \{u \in H^2(0,1) | u(0) = u'(0) = 0\}$. We decompose $a(u)$ as $a(u) = a_0(u) + \|Tu\|^2$ by defining

$$a_0(u) = \frac{a^2}{2}\int_0^1 (1 - y^2) \left| \frac{du}{dy} \right|^2 dy$$

with $\mathrm{Dom}(a_0) = \{u \in H^1(0,1) | u(0) = 0\}$, and

$$Tu = -\frac{d^2u}{dy^2}$$

with $\mathrm{Dom}(T)\{u \in H^2(0,1) | u(0) = u'(0) = 0\}$.

This decomposition corresponds to choosing the base operator to be the familiar Legendre operator:

$$A_0 = -\frac{a^2}{2}\frac{d}{dy}(1 - y^2)\frac{d}{dy}$$

with $\mathrm{Dom}\,(A_0) = \{u \in H^2(0,1) | u(0) = \lim_{\xi\to 1}(1-\zeta)u'(\xi) = 0\}$. This operator has explicitly known eigenvalues given by $\lambda_i^0 = a^2 i(2i-1)$ for $i = 1, 2, 3, \ldots$. The adjoint of T is computed to be $T^* = \frac{d^2}{dy^2}$ with $\mathrm{Dom}\,(T^*) = \{u \subset H^2(0,1) | u(1) = u'(1) = 0\}$.

We choose $\mu = 6.5_{10}4 = \lambda_{13}^0$ and finite-element bases for the two projecting subspaces involved. Cubic B-splines provide sufficient regularity in each case. For a mesh size of $1/N$ we produce subspaces of dimension $k = n = N$. Each submatrix in (3.4) is pentadiagonal, producing a sparse generalized matrix eigenvalue problem. Lower bounds using the EVF method of Sect. 3.3 with $N = 20$ and $N = 40$ were performed by G. Lee [25] and are listed in Table 3. Complementary Rayleigh-Ritz bounds were computed with cubic B-spline trial functions with $N = 50$.

Table 3. Eigenvalue bounds for rotating beam: $a^2 = 200$

Eigenvalue Index	A priori Lower bounds	Lower Bounds by EVF $N = 20$	$N = 40$	Rayleigh-Ritz Upper Bound ($N = 50$)
1	200	233.79343	233.79344	233.79349
2	1200	1771.6117	1771.6120	1771.6125
3	3000	7305.1301	7305.1611	7305.1685
4	5600	21714.896	21716.250	21716.393
5	9000	36707.188	51978.767	51983.742

6.2 Numerical realization

For the results presented above, we made no effort to exploit either the sparsity structure or the symmetry of the coefficient matrices and used the *QZ* method [29] to resolve the matrix eigenvalue problem (3.4). While extremely stable, such a direct approach, might be imprudent in larger problems where sparsity is significant.

A variety of computational approaches for the generalized matrix eigenvalue problem have been reviewed in [33]. Many of these require factorization of the Gram matrix $\begin{bmatrix} \mathscr{G}_1 & \mathscr{H} \\ \mathscr{H}^* & \mathscr{G}_2 \end{bmatrix}$ followed by either an implicit or explicit change of basis to obtain an eigenvalue problem in standard form. While such approaches may be inexpensive due to extensive sparsity in $\mathscr{G}_1$, $\mathscr{H}$, and $\mathscr{G}_2$, numerical stability may be at risk since in our experience $\begin{bmatrix} \mathscr{G}_1 & \mathscr{H} \\ \mathscr{H}^* & \mathscr{G}_2 \end{bmatrix}$ can be quite poorly conditioned or singular.

In fact, the matrix pencil (3.4) may not necessarily be diagonalizable (i.e., there may not exist any nonsingular matrix χ such that $\chi^* \cdot \mathscr{M}_{k,n}(\xi)\chi$ is diagonal). Consider, for a simple example, $T = (\lambda_1^0)^{-1/2} A_0$, $q_1 = p_1 = u_1^0$, and $\mu = 2\lambda_1^0$. For $k = n = 1$, (3.4) becomes

$$\begin{bmatrix} -\lambda_1^0 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \zeta \begin{bmatrix} (\lambda_1^0)^2 & -(\lambda_1^0)^{3/2} \\ -(\lambda_1^0)^{3/2} & \lambda_1^0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} ,$$

which is not diagonalizable. Thus any approach that involves (explicitly or implicitly) a reduction to a matrix eigenvalue problem in standard form must be used with caution. The spectral transformation Lanczos method as described in [30] may provide an attractive alternative that remains robust in the face of ill-conditioning (even singularity) of the Gram matrix, yet is able to produce partial results that still provide bounding information (cf. [11]).

7. Conclusions

We have introduced here a new approach for computing lower bounds to eigenvalues of self-adjoint operators that has greatly reduced requirements for a priori information over what is necessary for the Weinstein-Aronszajn methods or Temple-Lehmann methods, while combining to a great extent, their relative merits.

Our method is likely to be most useful in situations where problem geometry is complicated or domain dimension is large (e.g., as often occurs in quantum chemistry). In such situations the class of base problems for which full spectral information is both available and usable may be quite small (or even empty). By contrast, we require only a separating parameter (μ) in the base problem spectrum. No base problem eigenvector information is necessary nor are "exact" base problem eigenvalues needed. As may be seen from Example 2 of Sect. 6.1, a potentially important by-product of the elimination of base problem eigenvectors from the solution process is the possibility of using trial vectors with local support, producing as a consequence generalized matrix eigenvalue problems with well-structured sparsity that may then be exploited advantageously.

Appendix: Generalization of intermediate problem spectrum-slicing formulas

In [7], the following spectrum-slicing formula was shown to hold in general intermediate problem settings:

$$N_k(\lambda) = N_0(\lambda) - \mathbb{D}^-[\mathscr{W}^{\cdot}(\lambda)]$$

for all $\lambda \in \rho(A_0) \cap \rho(A_k)$, where $\rho(B)$ denotes the resolvent set of a linear operator B. The restriction to $\lambda \in \rho(A_0) \cap \rho(A_k)$ was convenient in [7], but is unduly constraining for the results we develop in the present paper. We will eliminate the restriction on λ, and provide generalizations of the spectrum-slicing formula of [7] for any λ below the first point of the essential spectrum for which $\mathscr{W}^{\cdot}(\lambda)$ is well-defined.

We first establish some continuity properties for inertias of W-A matrices.

Theorem A.1. *Suppose that* $\lambda^* < \inf\{\sigma_{\text{ess}}(A_0)\}$, $\{p_i\}_{i=1}^k$ *are linearly independent, and that* $\mathscr{W}(\lambda)$ *given by (2.3) is bounded at* $\lambda = \lambda^*$. *Then*

(*a*) $$\mathbb{D}^-[\mathscr{W}(\lambda^*)] = \lim_{\epsilon \to 0^+} \mathbb{D}^-[\mathscr{W}(\lambda^* + \epsilon)]$$

(*b*) $$\mathbb{D}^+[\mathscr{W}(\lambda^*)] = \lim_{\epsilon \to 0^+} \mathbb{D}^+[\mathscr{W}(\lambda^* - \epsilon)]$$

(*c*) $$\text{null}\,[\mathscr{W}(\lambda^*)] + \mathbb{D}^-[\mathscr{W}(\lambda^*)] = \lim_{\epsilon \to 0^+} \mathbb{D}^-[\mathscr{W}(\lambda^* - \epsilon)], \text{ and}$$

(*d*) $$\text{null}\,[\mathscr{W}(\lambda^*)] + \mathbb{D}^+[\mathscr{W}(\lambda^*)] = \lim_{\epsilon \to 0^+} \mathbb{D}^+[\mathscr{W}(\lambda^* + \epsilon)] .$$

Proof. Since $\mathscr{W}(\lambda^*)$ is bounded and the segments of $\sigma(A_k)$ and $\sigma(A_0)$ within which λ^* lies contain only isolated point spectra, there exists $\epsilon > 0$ such that $\mathscr{W}(\lambda)$ is continuous throughout the interval $(\lambda^* - \epsilon, \lambda^* + \epsilon)$. Furthermore, $\epsilon > 0$ may be chosen sufficiently small so that for $I_\ell \triangleq (\lambda^* - \epsilon, \lambda^*)$ and $I_\text{r} \triangleq (\lambda^*, \lambda^* + \epsilon)$, we have $I_\ell \cup I_\text{r} \subset \rho(A_0) \cap \rho(A_k)$.

By Aronszajn's Rule [1],

$$\mu_k(\lambda^*) = \mu_0(\lambda^*) + \text{null}\,[\mathscr{W}(\lambda^*)] ,$$

where $\mu_k(\lambda^*)$ and $\mu_0(\lambda^*)$ represent the respective multiplicity of λ^* as an eigenvalue of A_k and A_0. Now, pick $\lambda_\ell \in I_\ell$ and $\lambda_\text{r} \in I_\text{r}$ arbitrarily and observe from [7]

$$\mu_k(\lambda^*) = N_k(\lambda_\text{r}) - N_k(\lambda_\ell) = N_0(\lambda_\text{r}) - N_0(\lambda_\ell) + \mathbb{D}^-[\mathscr{W}(\lambda_\ell)] - \mathbb{D}^-[\mathscr{W}(\lambda_\text{r})] .$$

Since $\mu_0(\lambda^*) = N_0(\lambda_\text{r}) - N_0(\lambda_\ell)$, we find

$$\text{null}\,[\mathscr{W}(\lambda^*)] = \mathbb{D}^-[\mathscr{W}(\lambda_\ell)] - \mathbb{D}^-[\mathscr{W}(\lambda_\text{r})] .$$

Furthermore, since $\mathscr{W}(\lambda)$ is continuous in $(\lambda^* - \epsilon, \lambda^* + \epsilon)$ and $\text{null}\,[\mathscr{W}(\lambda)] = 0$ for all $\lambda \in I_\ell \cup I_\text{r}$, we can guarantee that $\mathbb{D}^-[\mathscr{W}(\lambda^*)] \geq \mathbb{D}^-[\mathscr{W}(\lambda_\text{r})]$ and $\mathbb{D}^+[\mathscr{W}(\lambda^*)] \geq \mathbb{D}^+[\mathscr{W}(\lambda_\ell)]$. Define the scalar $c = (\mathbb{D}^+[\mathscr{W}(\lambda^*)] - \mathbb{D}^+[\mathscr{W}(\lambda_\ell)] + (\mathbb{D}^-[\mathscr{W}(\lambda^*)] - \mathbb{D}^-[\mathscr{W}(\lambda_\text{r})])$ and note that $c \geq 0$ (being the sum of nonnegative quantities). Easy manipulation verifies that

$$\begin{aligned} c &= k - \mathbb{D}^+[\mathscr{W}(\lambda_\ell)] - \mathbb{D}^-[\mathscr{W}(\lambda_\text{r})] - (k - \mathbb{D}^+[\mathscr{W}(\lambda^*)]) - \mathbb{D}^-[\mathscr{W}(\lambda^*)]) \\ &= \mathbb{D}^-[\mathscr{W}(\lambda_\ell)] - \mathbb{D}^-[\mathscr{W}(\lambda_\text{r})] - \text{null}\,[\mathscr{W}(\lambda^*)] = 0 . \end{aligned}$$

Thus, $\mathbb{D}^-[\mathscr{W}(\lambda_\text{r})] = \mathbb{D}^-[\mathscr{W}(\lambda^*)]$ and $\mathbb{D}^+[\mathscr{W}(\lambda_\ell)] = \mathbb{D}^+[\mathscr{W}(\lambda^*)]$. Since λ_ℓ and λ_r were chosen arbitrarily within I_ℓ and I_r, respectively, conclusions (a) and (b) are true.

The conclusions (c) and (d) follow immediately upon the observation that

$$\mathbb{D}^-[\mathscr{W}(\lambda_\ell)] = \text{null}\,[\mathscr{W}(\lambda^*)] + \mathbb{D}^-[\mathscr{W}(\lambda_\text{r})]$$

and

$$\mathbb{D}^+[\mathscr{W}(\lambda_r)] = \operatorname{null}[\mathscr{W}(\lambda^*)] + \mathbb{D}^+[\mathscr{W}(\lambda_\ell)]\,. \qquad \square$$

The thrust of Theorem A.1 is that the positive and negative inertias of the W-A matrix are left- and right-continuous, respectively. Define $\tilde{N}_k(\lambda)$ to be the number of eigenvalues of A_k *less than or equal to* λ, with $\tilde{N}_0(\lambda)$ denoting the analogous quantity for A_0. We have

Theorem A.2. *Suppose* $\lambda^* < \inf\{\sigma_{\mathrm{ess}}(A_0)\}$, $\{p_i\}_{i=1}^k$ *are linearly independent, and that* $\mathscr{W}(\lambda)$ *is given by (2.3) is well defined at* $\lambda = \lambda^*$. *Then*

(*a*) $$\tilde{N}_k(\lambda^*) = \tilde{N}_0(\lambda^*) - \mathbb{D}^-[\mathscr{W}(\lambda^*)] \text{ and}$$

(*b*) $$N_k(\lambda^*) = N_0(\lambda^*) - \{\operatorname{null}[\mathscr{W}(\lambda^*)] + \mathbb{D}^-[\mathscr{W}(\lambda^*)]\}$$

Proof. $\mathscr{W}(\lambda)$ is continuous in an open interval containing λ^* and for all $\epsilon > 0$ sufficiently small, $(\lambda^* \pm \epsilon) \in \rho(A_0) \cap \rho(A_k)$. Observe that

$$\tilde{N}_k(\lambda^*) = \lim_{\epsilon \to 0^+} N_k(\lambda^* + \epsilon) \quad \text{and} \quad \tilde{N}_0(\lambda^*) = \lim_{\epsilon \to 0^+} N_0(\lambda^* + \epsilon)$$

whereas $N_k(\lambda^*) = \lim_{\epsilon \to 0^+} N_k(\lambda^* - \epsilon)$ and $N_0(\lambda^*) = \lim_{\epsilon \to 0^+} N_0(\lambda^* - \epsilon)$, in general. The spectrum-slicing results from [7] yield

$$N_k(\lambda^* \pm \epsilon) = N_0(\lambda^* \pm \epsilon) - \mathbb{D}^-[\mathscr{W}(\lambda^* \pm \epsilon)]$$

for all $\epsilon > 0$ sufficiently small. Taking $\epsilon \to 0$ and using A.1(a) and A.1(c) gives the conclusion. $\square$

Notice that A.2(a) may be obtained from A.2(b) (or vice versa) by adding (or subtracting) the multiplicity of λ^* as an eigenvalue of A_k as given by Aronszajn's Rule. We may relax the hypothesis of linear independence of $\{p_i\}_{i=1}^k$ to obtain finally:

Corollary. *If linear independence of* $\{p_i\}_{i=1}^k$ *is removed from the hypotheses of Theorem A.2 then the conclusion A.2(a) is unaffected and A.2(b) becomes*

(*b′*) $$N_k(\lambda^*) = N_0(\lambda^*) - \{\operatorname{null}[\mathscr{W}(\lambda^*)] + \mathbb{D}^-[\mathscr{W}(\lambda^*)]\} + \operatorname{null}[\langle p_i, p_j\rangle_*]\,.$$

Proof. Let $\alpha = k - \operatorname{null}[\langle p_i, p_j\rangle_*]$. A unitary matrix $\mathcal{Q} = [q_{ij}]$ may be found so that

$$\mathcal{Q}^*[\langle p_i, p_j\rangle_*]\mathcal{Q} = \begin{bmatrix} \mathscr{G} & 0 \\ 0 & 0 \end{bmatrix}$$

with $\mathscr{G} \in \mathbb{R}^{\alpha\times\alpha}$ nonsingular. Defining $\tilde{p}_j = \sum_{i=1}^{\alpha} q_{ij} p_i$ one may immediately observe that $\mathscr{G} = [\langle \tilde{p}_i, \tilde{p}_j\rangle_*]$, $\operatorname{span}_{i=1,\ldots,\alpha}\{\tilde{p}_i\} = \operatorname{span}_{i=1,\ldots,k}\{p_i\}$, and that $\{\tilde{p}_i\}_{i=1}^{\alpha}$ are linearly independent. Furthermore, if $\tilde{\mathscr{W}}(\lambda) = [\langle \tilde{p}_i, \tilde{p}_j\rangle_* + \langle R_\lambda^0 T^* \tilde{p}_i, T^* \tilde{p}_j\rangle]$ then $\mathscr{W}(\lambda)$ and $\tilde{\mathscr{W}}(\lambda)$ represent the same intermediate problem (2.2). Since $\mathcal{Q}^*\mathscr{W}(\lambda^*)\mathcal{Q} = \begin{bmatrix} \tilde{\mathscr{W}}(\lambda^*) & \theta \\ 0 & 0 \end{bmatrix}$, we have $\operatorname{null}[\mathscr{W}(\lambda^*)] = \operatorname{null}[\tilde{\mathscr{W}}(\lambda^*)] + \operatorname{null}[\langle p_i, p_j\rangle_*]$ and $\mathbb{D}^-[\mathscr{W}(\lambda^*)] = \mathbb{D}^-[\tilde{\mathscr{W}}(\lambda^*)]$. $\square$

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