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CONVERGENCE RATES FOR INTERMEDIATE PROBLEMS *

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Convergence rate estimates are derived for a variant of Aronszajn-type intermediate problems that is both computationally feasible and known to be convergent for problems with nontrivial essential spectrum. Implementation of these derived bounds is discussed in general and illustrated on differential eigenvalue problems. Convergence rates are derived for the commonly used method of simple truncation.

1. INTRODUCTION. The method of intermediate problems of Weinstein and Aronszajn provides a systematic way of generating improvable lower bounds to eigenvalues of self-adjoint operators. In a previous paper [6], we considered conditions sufficient to guarantee the convergence of these estimates for variations of the intermediate problem technique applied in settings that include nontrivial essential spectrum and relatively unbounded perturbations. Such settings occur in a great many quantum mechanical eigenvalue problems, for example. In this paper, we approach the related question of how fast this convergence can occur as a function of problem size.

Convergence rates for intermediate problems were first derived by Weinberger [21] for intermediate problems of constraint (Weinstein) type for a particular choice of approximating vectors. Somewhat later Fix [11], Birkhoff and Fix [8], and Poznyak [18, 19] obtained rate of convergence results for variants of Aronszajn's method with bounded or relatively bounded base operator perturbations.

In this paper we derive convergence rate estimates for a particular variant of Aronszajn's method known variously as "truncation including the remainder" [5, 6], or as "Aronszajn's method with a truncated base problem" [14]. This is the only method of Aronszajn type known to be both computationally

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feasible and convergent for problems with nontrivial essential spectra. The constructions involved with truncation including the remainder inevitably result in perturbations off the base operator that are not relatively bounded whenever the operator itself is unbounded, hence the previously known rate estimates are not applicable. It is useful to point out additionally that since Aronszajn's method with a truncated base problem is dominated by Aronszajn's method without truncation [4], we simultaneously obtain convergence rates for other variants of Aronszajn's method as well.

In Section 2, we review the main constructions and convergence results for intermediate problems of Aronszajn type incorporating truncation including the remainder. Criteria for exactness of estimates are introduced that directly motivate the convergence rate results. In Section 3, we derive convergence rate results under the hypothesis of boundedness for the operator of interest. We extend these results to the unbounded case in Section 4, and to the computationally practical case of simple truncation in Section 5. Finally in Section 6, we present a technique for implementing the convergence rate estimates that have been derived, and illustrate through applications to differential eigenvalue problems.

2. THE APPROXIMATION METHOD. The method we focus on is a variant of the original Aronszajn method of intermediate problems that was introduced in [4] and analyzed independently in [5] and [14] and in the later joint work [6]. The notation used here is adopted directly from [14].

Let $\mathcal{H}$ be a separable complex Hilbert space with norm $\| u \|$ and inner product $\langle u,v\rangle$. Let A be a self-adjoint operator on a domain $D(A)$ dense in $\mathcal{H}$. We suppose that A is bounded below with spectrum that begins with isolated eigenvalues of finite multiplicity,

$$\lambda_1(A) \leq \lambda_2(A) \leq \cdots \leq \lambda_\infty(A),$$

and corresponding orthonormal eigenvectors $u_1, u_2, \cdots$. Here $\lambda_\infty(A)$ denotes the lowest limit point of the spectrum of A. If A has compact resolvent, then by convention we set $\lambda_\infty(A) = \infty$. The closure of the quadratic form $\langle Au,u\rangle$ is denoted by $a(u)$.

To apply the method of intermediate problems, we require knowledge of another closed quadratic form, $a_0(u)$, satisfying $a_0(u) \leq a(u)$ for all $u \in D(a)$. Specifically, we require that the spectral problem for the self-adjoint operator A_0 corresponding to a_0 is solved explicitly and that the spectrum of A_0 also begins with isolated eigenvalues of finite multiplicity,

$$\lambda_1(A_0) \leq \lambda_2(A_0) \leq \cdots \leq \lambda_\infty(A_0),$$

with corresponding orthonormal eigenvectors u_1^0, $u_2^0, \cdots$. The second monotonicity theorem implies that $\lambda_\infty(A_0) \leq \lambda_\infty(A)$, and furthermore, for each i such that $\lambda_i(A) < \lambda_\infty(A_0)$, it is true that $\lambda_i(A_0)$ exists and $\lambda_i(A_0) \leq \lambda_i(A)$. Without loss of generality, we may assume that the difference between a_0 and a is strictly positive, that is

$$\hat{a}(u) = a(u) - a_0(u) \geq \alpha \parallel u \parallel^2,$$

for some $\alpha > 0$ and all $u \in D(a)$.

Now, pick a real parameter γ such that $\lambda_1(A_0) < \gamma \leq \lambda_\infty(A_0)$, with $\gamma < \lambda_\infty(A_0)$ if A_0 has an infinity of eigenvalues below $\lambda_\infty(A_0)$. Define the <u>truncation</u> <u>of</u> A_0 <u>at</u> γ, as

$$A_0^{(\gamma)} = A_0 E_{\gamma^-}[A_0] + \gamma(I - E_{\gamma^-}[A_0]) \tag{2.1}$$

where $E_\lambda[A_0]$ is the right continuous resolution of the identity for A_0. Observe that $A_0^{(\gamma)}$ has the same action as A_0 on the finite dimensional subspace,

$$\mathcal{U}_0^\gamma = R(E_{\gamma^-}[A_0]) = E_{\gamma^-}[A_0] \cdot \mathcal{H},$$

and acts as scalar multiplication by γ on vectors in $(\mathcal{U}_0^\gamma)^\perp$. The corresponding quadratic form, $a_0^{(\gamma)}$, may be used to define a second positive form,

$$\tilde{a}(u) = a(u) - a_0^{(\gamma)}(u) \geq \hat{a}(u) \geq \alpha \parallel u \parallel^2 .$$

One may easily observe that $D(\tilde{a}) = D(a)$, $\tilde{a}$ is a closed quadratic form, and the corresponding self-adjoint operator is given by $\tilde{A} = A - A_0^{(\gamma)}$ on $D(\tilde{A}) = D(A)$.

The method of approximation to be considered is simply Aronszajn's method with the truncated base operator $A_0^{(\gamma)}$, instead of the original base operator, A_0 (cf. [4, 14]). The method proceeds by selecting a set of trial vectors $\{p_i\}_{i=1}^\infty \subset D(\tilde{A})$ and defining for each n,

$$P_n u = \sum_{i,j=1}^{n} \langle u, \tilde{A}p_i \rangle b_{ij} p_j, \tag{2.2}$$

where $[b_{ij}]$ is the matrix inverse to $[\langle p_i, \tilde{A}p_j \rangle]_{i,j=1}^n$. It is an easy exercise to verify that P_n is the projection onto $\mathcal{P}_n = span_{i=1,\cdots,n}\{p_i\}$ that is orthogonal with respect to the inner product induced by $\tilde{a}$.

For each n, we define the intermediate form

$$a_n(u) = a_0^{(\gamma)}(u) + \tilde{a}(P_n u) \quad \text{for} \quad u \in D(a_n) = \mathcal{H}$$

with the corresponding self-adjoint operator

$$A_n = A_0^{(\gamma)} + \tilde{A} P_n.$$

Since the subspaces $\{P_n\}$ are nested and increasing with n, it follows from Bessel's inequality in the Hilbert space induced by $\tilde{a}$, that for all $u \in D(a)$,

$$a_0^{(\gamma)}(u) \le a_n(u) \le a_{n+1}(u) \le a(u).$$

For each i such that $\lambda_i(A) < \gamma$, the second monotonicity principle then provides

$$\lambda_i(A_0) = \lambda_i(A_0^{(\gamma)}) \le \cdots \le \lambda_i(A_{n+1}) \le \cdots \le \lambda_i(A).$$

Thus the intermediate operators, $\{A_n\}$, have eigenvalues that provide improving lower bounds to the eigenvalues of A as the index n is increased. For a discussion of methods to explictly compute intermediate operator eigenvalues see [3] or [24].

The first criteria for the convergence of Aronszajn's method were given by Aronszajn in 1951 [1] and later proved by Bazley and Fox in 1961 [2] for the case that both A and A_0 have compact resolvent and A is a relatively bounded perturbation of A_0. The general case allowing for the existence of essential spectra and unbounded perturbations was considered in detail in [5, 6, 9, 14]. We summarize the situation for our setting in the following theorem.

Theorem 2.1. *If the set of vectors $\{p_i\}_{i=1}^{\infty}$ is dense in $D(\tilde{A})$ with respect to the norm $\| \tilde{A}u \|$ then $\lim_{n\to\infty} \lambda_i(A_n) = \lambda_i(A)$ for each i satisfying $\lambda_i(A) < \gamma$, and $\liminf_{n\to\infty} \lambda_i(A_n) \ge \gamma$ for each i satisfying $\lambda_i(A) \ge \gamma$.*

One would expect that a particular choice of approximating vectors, $\{p_i\}_{i=1}^{n}$ exists that leads to exact estimates, i.e., $\lambda_i(A_n) = \lambda_i(A)$ for a <u>finite</u> index n.

Theorem 2.2. *Suppose the convergence criteria of Theorem 2.1 are satisfied. Define $\mathcal{U}^\gamma = R(E_{\gamma^-}[A])$. If, for all n sufficiently large,*

$$R(P_n) = \mathcal{P}_n \supset \mathcal{U}^\gamma, \tag{2.3}$$

then for sufficiently large n, $\lambda_i(A_n) = \lambda_i(A)$ *for each i such that* $\lambda_i(A) < \gamma$.

Proof. Define $\mathcal{U}_n^\lambda = R(E_{\lambda^-}[A_n])$ and let I be the largest index for which $\lambda_I(A) < \gamma$. Pick ϵ such that $0 < \epsilon < \gamma - \lambda_I(A)$. By Theorem 2.1, there exists a sufficiently large index N such that $n \geq N$ implies $\lambda_i(A_n) \geq \gamma - \epsilon$ for $i \geq I+1$. Thus for $n \geq N$, dim $\mathcal{U}_n^{\gamma-\epsilon} = I$.

Now pick $v \in \mathcal{U}^{\gamma-\epsilon}$ and observe that by hypothesis, (2.3) holds for $n \geq M$, for some $M > 0$. Hence for $n \geq max(N, M)$,

$$A_n v = A_0^{(\gamma)} v + \tilde{A} P_n v = A_0^{(\gamma)} v + \tilde{A} v = Av,$$

implying that A_n and A have the same action on $\mathcal{U}^{\gamma-\epsilon}$ and that

$$\lambda_i(A_n) = \lambda_i(A)$$

for $i = 1, ..., I$. ∎

Corollary. *If the convergence criteria of Theorem 2.1 hold and for all n sufficiently large,*

$$R(P_n^*) = \tilde{A}\mathcal{P}_n \supset span\{\mathcal{U}^\gamma, \mathcal{U}_0^\gamma\}, \tag{2.4}$$

then for sufficiently large n, $\lambda_i(A_n) = \lambda_i(A)$ *for each i such that* $\lambda_i(A) < \gamma$.

Proof. Observe first that $P_n^* = \tilde{A} P_n \tilde{A}^{-1}$. Now if $v \in \mathcal{U}^\gamma$, then $\tilde{A} v \in span\{\mathcal{U}^\gamma, \mathcal{U}_0^\gamma\}$. So for sufficiently large n

$$P_n^* \tilde{A} v = \tilde{A} v$$

implying that

$$P_n v = v$$

for all $v \in \mathcal{U}^\gamma$. Thus (2.3) holds. ∎

We are able to derive convergence rates by gauging the distance between an eigenvalue estimate $\lambda_i(A_n)$ and an exact eigenvalue $\lambda_i(A)$, in terms of a notion of separation between the approximating subspaces, $\tilde{A}\mathcal{P}_n$, and the "exact" subspaces, suggested by the Corollary to Theorem 2.2. The notion of distance between subspaces that we use we refer to as the <u>containment gap</u>, and is related to the usual notion of gap between subspaces [16].

Definition 2.3. Let $\mathcal{M}$ and $\mathcal{N}$ be two closed subspaces of $\mathcal{H}$ with $\dim \mathcal{N} > 0$. The containment gap between $\mathcal{M}$ and $\mathcal{N}$ is defined as

$$\delta_{\mathcal{N}}(\mathcal{M}) = \max_{0 \neq u \in \mathcal{N}} \frac{\| (I-Q)u \|}{\| u \|} = \| (I-Q)P \|,$$

where Q is the orthogonal projection onto $\mathcal{M}$ and P is the orthogonal projection onto $\mathcal{N}$.

Observe that $\delta_{\mathcal{N}}(\mathcal{M})$ is not symmetric in $\mathcal{N}$ and $\mathcal{M}$ (unlike the gap of [16]) and that $\delta_{\mathcal{N}}(\mathcal{M}) = 0$ if and only if $\mathcal{M} \supset \mathcal{N}$.

3. CONVERGENCE RATES FOR BOUNDED A. We use the truncation of A at γ, defined as

$$A^{(\gamma)} = AE_{\gamma^-}[A] + \gamma(I - E_{\gamma^-}[A]),$$

in order to introduce an auxiliary self-adjoint operator

$$A_n' = A_0^{(\gamma)} + P_n^*(A^{(\gamma)} - A_0^{(\gamma)})P_n,$$

where P_n is defined as in (2.2). Observe that the quadratic form, a_n', corresponding to A_n', satisfies

$$\begin{aligned} a_n'(u) &= a_0^{(\gamma)}(u) + a^{(\gamma)}(P_n u) - a_0^{(\gamma)}(P_n u) \\ &\leq a_0^{(\gamma)}(u) + a(P_n u) - a_0^{(\gamma)}(P_n u) = a_n(u). \end{aligned}$$

Thus the second monotonicity principle gives

$$\lambda_i(A_n') \leq \lambda_i(A_n) \leq \lambda_i(A) = \lambda_i(A^{(\gamma)})$$

for all i such that $\lambda_i(A) < \gamma$.

The importance of such a construction lies essentially in the fact that $A^{(\gamma)} - A_0^{(\gamma)}$ is compact. Now, if A is bounded, $\tilde{a}$ generates the topology of $\mathcal{H}$, so that under the convergence criteria of Theorem 2.1, $P_n \to I$ and $P_n^* \to I$, both in the strong operator topology. These observations are sufficient to conclude that $A_n' \to A^{(\gamma)}$ uniformly, implying in turn that

$$\lambda_i(A_n') \to \lambda_i(A) \qquad \text{and} \qquad \lambda_i(A_n) \to \lambda_i(A)$$

as $n \to \infty$ (cf. [14]). We refine these estimates here in order to derive convergence rates for $\lambda_i(A_n')$ which in turn imply convergence rates for $\lambda_i(A_n)$. For brevity, we refer to $\lambda_i(A_0)$ as λ_i^0 and $\lambda_i(A)$ as λ_i in what follows.

We proceed by decomposing A_n',

$$A_n' = E_n + B_n, \tag{3.1}$$

with

$$E_n u = \sum_k{}' (\lambda_k^0 - \gamma)[\langle u, u_k^0\rangle u_k^0 - \langle u, P_n^* u_k^0\rangle P_n^* u_k^0],$$

and

$$B_n u = \sum_k{}'' (\lambda_k - \gamma)\langle u, P_n^* u_k\rangle P_n^* u_k + \gamma u.$$

The single primed sum denotes that the summation is carried out over all k for which $\lambda_k^0 < \gamma$ and the double primed sum denotes that the summation is carried out over all k for which $\lambda_k < \gamma$. Since $P_n^* \to I$ strongly, it is evident from (3.1) that $E_n \to 0$ and $B_n \to A^{(\gamma)}$, both uniformly, as $n \to \infty$ (assuming the convergence criteria of Theorem 2.1).

Lemma 3.1. *We have*

$$\| E_n \| \leq (\gamma - \lambda_1^0)\alpha_1 \delta_{\mathcal{M}}(\tilde{A}\mathcal{P}_n)$$

where $\mathcal{M} = \mathcal{U}_0^\gamma$ *and* α_1 *is independent of* n.

Proof. From (3.1) we have

$$\begin{aligned}\| E_n \| &= \sup_{\|u\|=1} \| \sum{}' (\lambda_k^0 - \gamma)[\langle u, u_k^0 - P_n^* u_k^0\rangle u_k^0 + \langle u, P_n^* u_k^0\rangle (u_k^0 - P_n^* u_k^0)] \| \\ &\leq (\gamma - \lambda_1^0) \sum{}' (1 + \| P_n^* u_k^0 \|) \| u_k^0 - P_n^* u_k^0 \| .\end{aligned}$$

Since P_n is $\tilde{a}$-symmetric for each n, and $\tilde{a}$ is bounded, we have the uniform bound $\| P_n^* \| = \| P_n \| \leq \kappa$, where κ is the condition number of $\tilde{A}^{1/2}$, $\kappa = \| \tilde{A}^{1/2} \| \| \tilde{A}^{-1/2} \|$. We then obtain

$$\| E_n \| \leq (\gamma - \lambda_1^0) I_0 (1 + \kappa) \sup_{0 \neq u \in \mathcal{U}_0^\gamma} \frac{\| u - P_n^* u \|}{\| u \|},$$

where I_0 is the number of terms in the primed sum. Let Q_n be the orthogonal projection onto $R(P_n^*) = \tilde{A}\mathcal{P}_n$. Then

$$\| (I - P_n^*)u \| = \| (I - P_n^*)(I - Q_n)u \| \leq (1 + \kappa) \| (I - Q_n)u \|,$$

and so

$$\| E_n \| \leq (\gamma - \lambda_1^0) I_0 (1 + \kappa)^2 \sup_{0 \neq u \in \mathcal{U}_0^\gamma} \frac{\| (I - Q_n)u \|}{\| u \|}. \blacksquare$$

In a similar way we may obtain an estimate of the closeness of B_n to $A^{(\gamma)}$.

Lemma 3.2. *We have*

$$\| B_n - A^{(\gamma)} \| \leq (\gamma - \lambda_1)\alpha_2 \delta_{\mathcal{N}}[\tilde{A}\mathcal{P}_n]$$

where $\mathcal{N} = \mathcal{U}^\gamma$ *and* α_2 *is independent of* n.

Proof. Simply write

$$\begin{aligned} B_n u - A^{(\gamma)} u &= \sum\nolimits_k'' (\lambda_k - \gamma)[\langle u, P_n^* u_k\rangle P_n^* u_k - \langle u, u_k\rangle u_k] \\ &= \sum\nolimits_k'' (\lambda_k - \gamma)[\langle u, P_n^* u_k - u_k\rangle P_n^* u_k + \langle u, u_k\rangle (P_n^* u_k - u_k)]. \end{aligned}$$

Hence,

$$\| B_n u - A^{(\gamma)} u \| \leq \sum\nolimits_k'' |\lambda_k - \gamma| [\| u \| \| P_n^* u_k - u_k \| (1 + \| P_n^* u_k \|)]$$

and

$$\| B_n - A^{(\gamma)} \| \leq (\gamma - \lambda_1)(1+\kappa) \sum\nolimits_k'' \| P_n^* u_k - u_k \| .$$

As in Lemma 3.1 we proceed to find

$$\| B_n - A^{(\gamma)} \| \leq (\gamma - \lambda_1) I (1+\kappa)^2 \sup_{0 \neq u \in \mathcal{U}^\gamma} \frac{\| (I - Q_n) u \|}{\| u \|},$$

where I is the number of terms in the double primed sum.∎

It is easy to combine the estimates of Lemmas 3.1 and 3.2 to obtain error estimates.

Theorem 3.3. *If* a *is bounded then for each* i *such that* $\lambda_i(A) < \gamma$, *we have the estimates*

$$|\lambda_i(A) - \lambda_i(A_n)| \leq (\gamma - \lambda_1^0)\alpha_1 \delta_{\mathcal{M}}(\tilde{A}\mathcal{P}_n) + (\gamma - \lambda_1)\alpha_2 \delta_{\mathcal{N}}(\tilde{A}\mathcal{P}_n)$$

for $\mathcal{M} = \mathcal{U}_0^\gamma$ *and* $\mathcal{N} = \mathcal{U}^\gamma$.

Proof. Since $\lambda_i(A_n') \leq \lambda_i(A_n) \leq \lambda_i(A)$ we have

$$\begin{aligned} |\lambda_i(A) - \lambda_i(A_n)| &\leq |\lambda_i(A) - \lambda_i(A_n')| \\ &\leq \| A_n' - A^{(\gamma)} \| \leq \| E_n \| + \| B_n - A^{(\gamma)} \| . \end{aligned}$$ ∎

4. EXTENSION TO UNBOUNDED A. A number of technical difficulties arise for the estimates of Theorem 3.3 when A is unbounded. To begin with, $\tilde{A}$ is then unbounded as well and so, it could happen that P_n fails to converge strongly to I so that $\{P_n\}$ may not be uniformly bounded. The preceding arguments then fail to produce necessarily finite constants for α_1 and α_2 in our estimates.

We are able to bypass these difficulties by using the device of [14] in introducing the auxiliary operator

$$\tilde{\tilde{A}} = A^{(\mu)} - A_0^{(\gamma)},$$

where μ is chosen sufficiently large so that the corresponding quadratic form satisfies $\tilde{\tilde{a}}(u) \geq (\frac{\alpha}{2}) \parallel u \parallel^2$, with α as in Section 2. See [14] for a proof that such a μ necessarily exists. We have then

$$a^{(\mu)}(u) = a_0^{(\gamma)}(u) + \tilde{\tilde{a}}(u),$$

and we apply Aronszajn's method to this decomposition of $a^{(\mu)}$ in the following way.

Given the approximating vectors $\{p_i\}_{i=1}^{\infty}$, generate $\{\hat{p}_i\}_{i=1}^{\infty}$ by $\hat{p}_i = \tilde{\tilde{A}}^{-1}\tilde{A}p_i$ for each $i = 1, 2, \cdots$. Define projections onto $\hat{\mathcal{P}}_n = span_{i=1,\cdots,n}\{\hat{p}_i\}$ by

$$\hat{P}_n u = \sum_{i,j=1}^{n} \langle u, \tilde{\tilde{A}}\hat{p}_i\rangle \hat{b}_{ij}\hat{p}_j$$

where $[\hat{b}_{ij}]$ is the matrix inverse to $[\langle \hat{p}_i, \tilde{\tilde{A}}\hat{p}_j\rangle]$. Observe that $\hat{P}_n$ is an orthogonal projection with respect to the inner product induced by $\tilde{\tilde{a}}(u)$. Furthermore, for each n, $R(I - \hat{P}_n) = Ker\hat{P}_n = KerP_n = R(I - P_n)$, where $KerP_n$ denotes the kernel of P_n, and $\tilde{\tilde{A}}\hat{\mathcal{P}}_n \equiv \tilde{A}\mathcal{P}_n$. Define intermediate operators

$$A_n'' = A_0^{(\gamma)} + \tilde{\tilde{A}}\hat{P}_n.$$

Our construction implies that $\lambda_i(A_n'') \leq \lambda_i(A_n) \leq \lambda_i(A)$ for each i such that $\lambda_i(A) < \gamma$. In fact since $\hat{P}_n$ is orthogonal with respect to $\tilde{\tilde{a}}(u,v)$, we have for $u \in D(\tilde{a})$,

$$\begin{aligned} \tilde{\tilde{a}}(\hat{P}_n u) &= \tilde{\tilde{a}}(u - (I - \hat{P}_n)u) \leq \tilde{\tilde{a}}(u - (I - P_n)u) \\ &= \tilde{\tilde{a}}(P_n u) \leq \tilde{a}(P_n u) \leq \tilde{a}(u). \end{aligned}$$

The desired generalization of Theorem 3.3 comes directly now.

Theorem 4.1. *For each i such that $\lambda_i(A) < \gamma$ we have*

$$|\lambda_i(A) - \lambda_i(A_n)| \leq (\gamma - \lambda_1^0)\alpha_1 \delta_{\mathcal{M}}(\tilde{A}\mathcal{P}_n) + (\gamma - \lambda_1)\alpha_2 \delta_{\mathcal{N}}(\tilde{A}\mathcal{P}_n),$$

where $\mathcal{M} = \mathcal{U}_0^\gamma$ and $\mathcal{N} = \mathcal{U}^\gamma$.

Proof. The bounded case has been considered in Section 3. Suppose A is unbounded. We first construct $\tilde{\tilde{A}}$ and $\{A_n''\}$ as specified above and observe that it is sufficient to estimate $|\lambda_i(A^{(\mu)}) - \lambda_i(A_n'')|$. Since $A^{(\mu)}$ and $\tilde{\tilde{A}}$ are bounded, Theorem 3.3 implies

$$|\lambda_i(A^{(\mu)}) - \lambda_i(A_n'')| \leq (\gamma - \lambda_1^0)\alpha_1 \delta_{\mathcal{M}}(\tilde{\tilde{A}}\hat{\mathcal{P}}_n) + (\gamma - \lambda_1)\alpha_2 \delta_{\mathcal{N}}(\tilde{\tilde{A}}\hat{\mathcal{P}}_n).$$

The conclusion follows, since by construction $\tilde{\tilde{A}}\hat{\mathcal{P}}_n = \tilde{A}\mathcal{P}_n$.∎

5. SIMPLE TRUNCATION. Following the constructions of Section 2, suppose that the operator A has the decomposition

$$A = A_0 + \hat{A},$$

where $\hat{A}$ is a positive symmetric operator. In particular, $D(A) \subset D(A_0)$. We select vectors $\{p_i\}_{i=1}^{\infty} \subset D(\hat{A})$ and define

$$R_n u = \sum_{i,j=1}^{n} \langle u, \hat{A}p_i \rangle b_{ij} p_j,$$

where $[b_{ij}]$ is the matrix inverse to $[\langle p_i, \hat{A}p_j \rangle]$. Pick an integer ν so that $\lambda_{\nu+1}^0 > \lambda_\nu^0$ and let A_0^ν represent the truncation of A_0 at $\lambda_{\nu+1}^0$. Define a doubly indexed family of intermediate operators by

$$A_n^\nu = A_0^\nu + \hat{A}R_n.$$

This differs from the intermediate operators we formed in section 2 in that we omit the truncation remainder $A_0 - A_0^\nu$ from $\tilde{A}$. Hence the projections R_n here are independent of ν, whereas in section 2, P_n did depend on the truncation point.

The notion of the spectral truncation of an operator was originally developed in order to reduce the Weinstein-Aronszajn perturbation determinant to a rational function in finite form (cf. [2, 22]). This idea forms the basis of a number of numerical schemes for computing tight lower bounds to operator eigenvalues (cf. [3, 23]), and was shown to be convergent in [2] for operators without essential spectra when $\hat{A}$ is bounded relative to A_0.

Defining $A^\nu = A_0^\nu + \hat{A}$, we have from Theorem 4.1 the following lemma.

Lemma 5.1. *For each i such that $\lambda_i(A) < \lambda_{\nu+1}^0$ we have*

$$|\lambda_i(A^\nu) - \lambda_i(A_n^\nu)| \le (\lambda_{\nu+1}^0 - \lambda_1^0)\alpha_1\delta_{\mathcal{M}}[\hat{A}\mathcal{R}_n] + (\lambda_{\nu+1}^0 - \lambda_1)\alpha_2\delta_{\mathcal{N}}[\hat{A}\mathcal{R}_n]$$

where $\mathcal{M} = \mathcal{U}_0^\tau$ and $\mathcal{N} = R(E_{\tau^-}[A^\nu])$ with $\tau = \lambda_{\nu+1}^0$, and $\mathcal{R}_n = R_n \cdot H$.

In order to obtain a rate estimate on $|\lambda_i(A) - \lambda_i(A_n^\nu)|$, it remains only to estimate $|\lambda_i(A) - \lambda_i(A^\nu)|$. Without loss of generality we assume that A and A_0 are positive definite.

Lemma 5.2. *For each i such that $\lambda_i(A) < \lambda_{\nu+1}^0$,*

$$|\lambda_i(A) - \lambda_i(A^\nu)| \le \alpha_3 \frac{[\lambda_i(A)]^2}{(\lambda_{\nu+1}^0)^{1/2}},$$

where α_3 is independent of ν.

Proof. Evidently,

$$|1/\lambda_i(A) - 1/\lambda_i(A^\nu)| \le \| A^{-1} - (A^\nu)^{-1} \| .$$

Since $D(A) \subset D(A_0)$,

$$A - A^\nu \subset A_0 - A_0^\nu$$

and

$$A^\nu[A^{-1} - (A^\nu)^{-1}]A \subset A_0^\nu[A_0^{-1} - (A_0^\nu)^{-1}]A_0,$$

where $\subset$ indicates that the operator on the right extends that on the left.

Thus we have

$$A^{-1} - (A^\nu)^{-1} = (A^\nu)^{-1}A_0^\nu[A_0^{-1} - (A_0^\nu)^{-1}]A_0A^{-1}.$$

Since $R(A^{-1}) = D(A) \subset D(A_0)$, A_0A^{-1} is bounded. A bound on the term $(A^\nu)^{-1}A_0^\nu$ may be obtained by first writing

$$(A^\nu)^{-1}A_0^\nu = (A^\nu)^{-1/2}[(A^\nu)^{-1/2}(A_0^\nu)^{1/2}](A_0^\nu)^{1/2}.$$

Now, $\| (A^\nu)^{-1/2} \| \le \| (A_0^\nu)^{-1/2} \| = 1/(\lambda_1^0)^{1/2}$. The bracketed expression is bounded by 1 uniformly in ν since $A_0^\nu \le A^\nu$. Finally, $\| (A_0^\nu)^{1/2} \| = (\lambda_{\nu+1}^0)^{1/2}$. Thus,

$$\| A^{-1} - (A^\nu)^{-1} \| \le \left(\frac{\lambda_{\nu+1}^0}{\lambda_1^0}\right)^{1/2} \| A_0^{-1} - (A_0^\nu)^{-1} \| \| A_0A^{-1} \| = \frac{\alpha_3}{(\lambda_{\nu+1}^0)^{1/2}},$$

where $\alpha_3 = \| A_0 A^{-1} \| / (\lambda_1^0)^{1/2}$. We may conclude that

$$\lambda_i(A)\lambda_i(A^\nu)|1/\lambda_i(A) - 1/\lambda_i(A^\nu)| \leq \alpha_3 \frac{\lambda_i(A)\lambda_i(A^\nu)}{(\lambda_{\nu+1}^0)^{1/2}}$$

or

$$|\lambda_i(A^\nu) - \lambda_i(A)| \leq \alpha_3 \frac{[\lambda_i(A)]^2}{(\lambda_{\nu+1}^0)^{1/2}}. \blacksquare$$

Lemmas 5.1 and 5.2 may now be combined. The following theorem proves convergence of simple truncation, and estimates the rate of convergence, if also A_0 has compact inverse.

Theorem 5.3. *For each i such that $\lambda_i(A) < \lambda_{\nu+1}^0$,*

$$|\lambda_i(A) - \lambda_i(A_n^\nu)| \leq (\gamma - \lambda_1^0)\alpha_1 \delta_{\mathcal{M}}[\hat{A}\mathcal{R}_n] + (\gamma - \lambda_1)\alpha_2 \delta_{\mathcal{N}}[\hat{A}\mathcal{R}_n] + \alpha_3 \frac{[\lambda_i(A)]^2}{(\lambda_{\nu+1}^0)^{1/2}}$$

were $\mathcal{M} = \mathcal{U}_0^\tau$ and $\mathcal{N} = R(E_{\tau^-}[A^\nu]$ with $\tau = \lambda_{\nu+1}^0$.

6. APPLICATIONS. In order to apply the preceding estimates to differential eigenvalue problems, we first introduce a convenient means of dominating $\| u - Q_n u \|$ in terms of the spectral projections of an auxiliary operator $\mathbf{B}$. Now Q_n is the orthogonal projection in $\mathcal{H}$ onto $R(P_n^*)$, thus if the elements $\{p_k\}$ are chosen so that the vectors $\{\tilde{A}p_k\}$ are orthonormal in $\mathcal{H}$,

$$Q_n u = \sum_{k=1}^{n} \langle u, \tilde{A}p_k \rangle \tilde{A}p_k, \qquad u \in \mathcal{H}.$$

Then the vectors p_k are orthonormal in the Hilbert space $D(\tilde{A})$ provided with the norm $\| \tilde{A}u \|$, $u \in D(A)$, and the orthogonal projection, $\tilde{Q}_n$, in this space onto $span\{p_1, \cdots, p_n\}$ is given by

$$\tilde{Q}_n u = \sum_{k=1}^{n} \langle \tilde{A}u, \tilde{A}p_k \rangle p_k, \qquad u \in D(\tilde{A}).$$

Thus for $u \in \mathcal{H}$,

$$\begin{aligned} u - Q_n u &= \tilde{A}(\tilde{A}^{-1}u - \sum_{k=1}^{n} \langle \tilde{A}(\tilde{A}^{-1}u), \tilde{A}p_k \rangle p_k) \\ &= \tilde{A}(I - \tilde{Q}_n)\tilde{A}^{-1}u. \end{aligned}$$

Now let $\mathbf{B}$ be a positive definite self adjoint operator in $\mathcal{H}$ such that $D(\mathbf{B}) \subset D(\tilde{A})$ and $\| \tilde{A}u \| \leq \beta \| \mathbf{B}u \|$, $\beta > 0$, for all $u \in D(\mathbf{B})$. Further suppose that the vectors p_k have been chosen to be eigenvectors of $\mathbf{B}$ and let $\mathbf{Q}_n$ be the orthogonal projection in $\mathcal{H}$ onto $span\{p_1, \cdots, p_n\}$. Then $\mathbf{B}$ commutes with $\mathbf{Q}_n$ and for any $u \in \mathcal{H}$ such that $\tilde{A}^{-1}u \in D(\mathbf{B})$,

$$\begin{aligned}
\| u - Q_n u \| &= \| \tilde{A}(I - \tilde{Q}_n)\tilde{A}^{-1}u \| \\
&= \| \tilde{A}(I - \tilde{Q}_n)(I - \mathbf{Q}_n)\tilde{A}^{-1}u \| \\
&\leq \| \tilde{A}(I - \mathbf{Q}_n)\tilde{A}^{-1}u \| \\
&\leq \beta \| \mathbf{B}(I - \mathbf{Q}_n)\tilde{A}^{-1}u \| \\
&\leq \beta \| (I - \mathbf{Q}_n)\mathbf{B}\tilde{A}^{-1}u \| .
\end{aligned}$$

So assume that $\mathbf{B}^{-1}$ is compact and let

$$0 < \mu_1 \leq \mu_2 \leq \cdots \leq \mu_k \cdots \nearrow \infty$$

be the eigenvalues of $\mathbf{B}$ enumerated as usual according to multiplicity, with corresponding eigenvectors $\{p_k\}$ orthonormal in $\mathcal{H}$. Let $w = \tilde{A}^{-1}u$ and assume that $w \in D(\mathbf{B}^\tau)$ with $\tau > 1$. Then

$$\begin{aligned}
\| (I - \mathbf{Q}_n)\mathbf{B}w \|^2 &= \sum_{k=n+1}^{\infty} \mu_k^2 |\langle p_k, w\rangle|^2 \\
&= \sum_{k=n+1}^{\infty} \mu_k^2 |\langle \mathbf{B}^{-\tau} p_k, \mathbf{B}^\tau w\rangle|^2 \\
&= \sum_{k=n+1}^{\infty} \mu_k^{2-2\tau} |\langle p_k, \mathbf{B}^\tau w\rangle|^2 \\
&\leq \mu_{n+1}^{2-2\tau} \sum_{k=n+1}^{\infty} |\langle p_k, \mathbf{B}^\tau w\rangle|^2 \\
&= o(\mu_{n+1}^{2-2\tau}) \quad \text{as} \quad n \to \infty,
\end{aligned}$$

where o is the usual Landau symbol. Thus if $\tau > 1$ and $\tilde{A}^{-1}u \in D(\mathbf{B}^\tau)$,

$$\text{(6.1)} \qquad \| (I - \mathbf{Q}_n)\mathbf{B}\tilde{A}^{-1}u \| = o(\mu_{n+1}^{1-\tau}) \quad \text{as} \quad n \to \infty.$$

To implement this estimate first note that

$$\tilde{A} = (A - \gamma) + \sum_i{}' (\gamma - \lambda_i^0)\langle u, u_i^0\rangle u_i^0.$$

In particular, $\tilde{A}$ is a finite rank perturbation of $A - \gamma$. We may also assume that γ is not an eigenvalue of A, without loss of generality. Then the following formula expresses $\tilde{A}^{-1}$ in terms of $(A-\gamma)^{-1}$: for $u \in \mathcal{H}$,

$$\begin{aligned}\tilde{A}^{-1}u &= (A-\gamma)^{-1}u \\ &\quad - {\sum_{i,j}}' \langle u, (A-\gamma)^{-1}u_i^0\rangle (\gamma - \lambda_i^0)^{1/2} c_{ij} (\gamma - \lambda_j^0)^{1/2} (A-\gamma)^{-1} u_j^0,\end{aligned}$$

where $'$ now denotes summation over all indices i, j such that λ_i^0 and λ_j^0 are both less than γ, and $[c_{ij}]$ is the matrix inverse to

$$[\delta_{ij} + (\gamma - \lambda_i^0)^{1/2}(\gamma - \lambda_j^0)^{1/2}\langle u_i^0, (A-\gamma)^{-1}u_j^0\rangle].$$

Herein δ_{ij} is the Kronecker symbol.

Hence we see that if for all λ_j and λ_j^0 less than γ, both u_j and $(A-\gamma)^{-1}u_j^0$ are in $D(\mathbf{B}^\tau)$ with $\tau > 1$, (6.1) and Theorem 4.1 imply that

$$|\lambda_i(A) - \lambda_i(A_n)| = o(\mu_{n+1}^{1-\tau}) \quad \text{as} \quad n \to \infty.$$

Theorem 5.3 also yields a corresponding estimate in the case of simple truncation.

As an example, let Ω be a bounded domain in $\mathbf{R}^2$, $\mathcal{H} = L^2(\Omega)$ and, for $u \in H_0^1(\Omega)$ — the closure of $C_0^\infty(\Omega)$ in the Sobolev space $H^1(\Omega)$ — let

$$a(u) = \int_\Omega (|\text{grad } u|^2 + q|u|^2)dx,$$

where q is a smooth non-negative function on $\overline{\Omega}$. We further assume that Ω is locally similar by $C^{1,1}$ homeomorphsisms to a convex domain so that the regularity results of Kadlec [15] imply that $D(A) = H^2(\Omega) \cap H_0^1(\Omega)$. Note that this means

$$Au = -\Delta u + qu \quad \text{in} \quad \Omega, \qquad u = 0 \quad \text{on} \quad \partial\Omega,$$

where Δ is the Laplace operator. Let

$$a_0(u) = \int_\Omega |\text{grad } u|^2 dx, \qquad u \in H_0^1(\Omega),$$

i.e.,

$$A_0 u = -\Delta u \quad \text{in} \quad \Omega, \qquad u = 0 \quad \text{on} \quad \partial\Omega,$$

and further assume that Ω is such that the eigenvalue problem for A_0 is explicitly solvable. To implement the estimate (6.1), let $\mathbf{B} = A_0$ so that $p_k = u_k^0$ and $\mu_k = \lambda_k^0$. Then

$$\mathbf{B}u_j = A_0 u_j = \lambda_j u_j - q u_j \in H^2(\Omega) \cap H_0^1(\Omega),$$

and so

$$A_0^2 u_j = (\lambda_j - q)^2 u_j + (\Delta q) u_j + 2 \text{ grad } q \cdot \text{grad } u_j \in H^1(\Omega),$$

so that $u_j \in D(\mathbf{B}^\tau) = D(A_0^\tau)$ for all $\tau < 9/4$ (cf. [12]). In addition,

$$A_0(A-\gamma)^{-1}u_j^0 = u_j^0 + (\gamma - q)(A-\gamma)^{-1}u_j^0 \in H^2(\Omega) \cap H_0^1(\Omega),$$

and

$$\begin{aligned} A_0^2(A-\gamma)^{-1}u_j^0 = {} & (\lambda_j^0 + \gamma - q)u_j^0 + (\Delta q)(A-\gamma)^{-1}u_j^0 \\ & + 2 \text{ grad } q \cdot \text{grad}((A-\gamma)^{-1}u_j^0) \\ & + (\gamma - q)^2 (A-\gamma)^{-1}u_j^0 \in H^1(\Omega), \end{aligned}$$

so that $(A-\gamma)^{-1}u_j^0 \in D(A_0^\tau)$ for all $\tau < 9/4$. Thus since $\lambda_n^0 \sim$ (constant) n as $n \to \infty$ (cf. [10]), (6.1) and Theorem 4.1 imply that

$$|\lambda_i(A) - \lambda_i(A_n)| = o(n^{-\tau}) \quad \text{as} \quad n \to \infty \quad \text{for all} \quad \tau < 5/4.$$

If also grad $q = 0$ on $\partial\Omega$, then $A_0^2 u_j$ and $A_0^2(A-\gamma)^{-1}u_j^0$ are in $H_0^1(\Omega)$ so that u_j and $(A-\gamma)^{-1}u_j^0$ are in $D(A_0^{5/2})$. Hence

$$|\lambda_i(A) - \lambda_i(A_n)| = o(n^{-3/2}) \quad \text{as} \quad n \to \infty.$$

If, in addition, $\partial\Omega$ is smooth, then $A_0^2 u_j$ and $A_0^2(A-\gamma)^{-1}u_j^0$ are also smooth on $\overline{\Omega}$ (cf. [17]) so that u_j and $(A-\gamma)^{-1}u_j^0$ are in $D(A_0^\tau)$ for all $\tau < 13/4$. In this case,

$$|\lambda_i(A) - \lambda_i(A_n)| = o(n^{-\tau}) \quad \text{as} \quad n \to \infty \quad \text{for all} \quad \tau < 9/4.$$

More rapid rates of convergence now follow from further special conditions on q near $\partial\Omega$.

As a second example we estimate the rate of convergence in a differential problem with non-trivial continuous spectrum—the first such estimate of which we are aware. We consider an eigenvalue problem for the radial equation of quantum mechanics at zero angular momentum. As potential we take a "potential well" function, q, which is smooth on $[0,\infty)$ with $q(0) < 0$ and such that:

(6.2) q is strictly increasing on $[0, x_1]$ to a positive maximum at x_1;

(6.3) q is decreasing on $[x_1, \infty)$ with $q(x)$, $q'(x)$, $q''(x)$, and $q'''(x)$ tending to zero as $x \to \infty$; and

(6.4) $q \in L^2(0,\infty)$.

Hypotheses (6.2) and (6.3) can readily be relaxed, but are consistent with typical potential well considerations, and ease the exposition.

Now for $u \in H_0^1(0,\infty)$, let

$$a(u) = \int_0^\infty (|u'|^2 + q|u|^2)dx.$$

Then with $\mathcal{H} = L^2(0,\infty)$, $D(A) = H^2(0,\infty) \cap H_0^1(0,\infty)$, and the eigenvalue problem for A means,

$$-u'' + qu = \lambda u \quad \text{on} \quad (0,\infty), \quad u(0) = 0, \quad u \in L^2(0,\infty).$$

We assume that the potential well is "deep enough" that A has at least one negative eigenvalue.

An explicitly solvable lower bound problem is obtained from

$$-u'' + q_0 u = \lambda u \quad \text{on} \quad (0,\infty), \quad u(0) = 0, \quad u \in L^2(0,\infty),$$

with q_0 the "square well" potential:

$$q_0(x) = \begin{cases} q(0) + \gamma, & 0 \le x < x_0, \\ \gamma, & x > x_0. \end{cases}$$

Herein x_0 is the unique zero of q, i.e., $q(x_0) = 0$, and $\gamma < 0$ is great enough that all negative eigenvalues of A are less than γ. The negative number γ will, as previously, be our truncation point—and has been added to the usual square well potential so that $\hat{a}(u)$, and therefore $\tilde{a}(u)$, are positive definite. This eigenvalue problem is obtained from the quadratic form,

$$a_0(u) = \int_0^\infty (|u'|^2 + q_0|u|^2)dx, \quad u \in H_0^1(0,\infty),$$

and $D(A_0) = D(A) = H^2(0,\infty) \cap H_0^1(0,\infty)$.

To implement the estimate (6.1), let $\mathbf{B}$ be the harmonic oscillator operator with Dirichlet boundary condition at zero, i.e.,

$$\mathbf{B} = -\frac{d^2}{dx^2} + x^2,$$

with $D(\mathbf{B}) = H^2(0,\infty) \cap H_0^1(0,\infty) \cap D(x^2)$. As usual, $D(x^2) = \{u \in L^2(0,\infty)$: $\int_0^\infty x^4 u^2(x)dx < \infty\}$. Then $\mathbf{B}$ is self-adjoint on $D(\mathbf{B})$ (cf. [20]), and $\mu_k = 4k-1$. Now since $u_j \in H_0^1(0,\infty)$ it follows from (6.3), (6.4), and [7] that

$$\begin{aligned} |u_j(x)| &= \mathcal{O}(\exp[-|\lambda_j|^{1/2}x \\ &\quad - (1/2|\lambda_j|^{1/2}) \int_0^x q(y)dy + o(1)]) \quad \text{as} \quad x \to \infty. \end{aligned} \tag{6.5}$$

Thus an application of the Cauchy-Schwartz inequality to $1 \cdot q(y)$ in the integral in (6.5) establishes that u_j decays exponentially as $x \to \infty$. The analogous estimate holds for u_j^0. Now the differential equation

$$-\psi'' + (q(x) - \gamma)\psi = 0, \quad x \in (0,\infty),$$

has solutions ψ_1 and ψ_2 satisfying,

$$\psi_1(x) = \exp[|\gamma|^{1/2} + (1/2|\gamma|^{1/2}) \int_0^x q(y)dy + o(1)] \quad \text{as} \quad x \to \infty,$$

and,

$$\psi_2(x) = \exp[-|\gamma|^{1/2}x - (1/2|\gamma|^{1/2}) \int_0^x q(y)dy + o(1)] \quad \text{as} \quad x \to \infty$$

(cf. [7]). Use of ψ_1 and ψ_2 to construct the Green's function for $A - \gamma$ establishes that

$$|[(A-\gamma)^{-1}u_j^0](x)| = \mathcal{O}(\exp[(\epsilon - |\lambda_j^0|^{1/2})x]) \quad \text{as} \quad x \to \infty,$$

where $\epsilon > 0$ is arbitrarily small.

It now follows by the methods of the preceding example and the identity,

$$\begin{aligned} \frac{d}{dx}[(A-\gamma)^{-1}u_j^0](x) &= -\int_x^\infty \frac{d^2}{dy^2}[(A-\gamma)^{-1}u_j^0](y)dy \\ &= -\int_x^\infty (1 + q(y) - \gamma)u_j^0(y)dy, \end{aligned}$$

that $\mathbf{B}^2 u_j \in H^1(0,\infty) \cap D(x^2)$, and that $\mathbf{B}^2(A-\gamma)^{-1}u_j^0 \in H^\tau(0,\infty) \cap D(x^2)$ for all $\tau < 1/2$. Thus by [13], both u_j and $(A-\gamma)^{-1}u_j^0$ are in $D(\mathbf{B}^\tau)$ for all $\tau < 9/4$. Hence (6.1) and Theorem 4.1 imply that

$$|\lambda_i(A) - \lambda_i(A_n)| = o(n^{-\tau}) \quad \text{as} \quad n \to \infty \quad \text{for all} \quad \tau < 5/4.$$

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