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ON THE METHOD OF LEAST SQUARES OF FINDING EIGENVALUES
AND EIGENFUNCTIONS OF SOME SYMMETRIC OPERATORS, II

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In [1], we studied the method of least squares for approximating the eigenvalues of a DS-operator. From the results of [1] it follows that the approximation $\lambda^{(n)}$ to an eigenvalue λ depends on a parameter μ , i.e., $\lambda^{(n)} = \lambda^{(n)}(\mu)$ and we can obtain upper or lower bounds of λ for appropriate choice of μ . In this paper, we shall consider the problem of the optimum choice of the μ which leads to an error $\lambda^{(n)}(\mu) - \lambda$ of minimum absolute value. For the case in which A is a bounded below operator we shall show that the Ritz's approximation to the smallest eigenvalue of A is "a limit's case" of the approximations obtained from applying the method of least squares. Finally, we shall consider the problem of approximating the eigenfunctions of a DS-operator using the method of least squares.

We assume throughout that A be a DS-operator with its domain a real separable Hilbert space H , i.e., A is a symmetric operator in H such that the set of its eigenvalues is of the first category on the real a-

xis and the spectrum $\sigma(A)$ is the closure of this set. Let $\lambda_i, i = 1, 2, \dots$ be an enumeration of distinct eigenvalues of A . Further, we assume that $\{\Psi_i\}_{i=1}^{\infty}$ is a totally complete system.

1. In this section we shall consider the problem of the optimum choice of μ . Let $\lambda^{(n)}(\mu)$ be defined by

$$(1) \lambda^{(n)}(\mu) = \begin{cases} \mu + q_n(\mu) & \text{for } \mu < \lambda_j, \\ \mu - q_n(\mu) & \text{for } \mu > \lambda_j, \end{cases}$$

where

$$(2) \quad q_n(\mu) = \min_{\substack{u \in \mathcal{L}\{\Psi_i\}_{i=1}^n \\ u \neq 0}} \frac{\|Au - \mu u\|}{\|u\|}$$

and λ_j is a fixed eigenvalue of A .

We remark that $\lim_{n \rightarrow \infty} q_n = \inf_{t \in \sigma(A)} |t - \mu|$ (Theorem 3 of [1], p.318). Before proving Theorem 1, we establish the following lemma.

Lemma 1. The function $\lambda^{(n)}(\mu)$ is monotone increasing in each of the intervals $I_1 = (-\infty, \lambda_j)$ and $I_2 = (\lambda_j, +\infty)$.

Proof. Firstly, assume that $\mu_0 < \mu_1, \mu_1 \in I_1$. It follows from the definition of $q_n(\mu)$ in (2) that there exists $u_1 \in \mathcal{L}\{\Psi_i\}_{i=1}^n$ such that $\|u_1\| = 1$ and $q_n(\mu_1) = \|Au_1 - \mu_1 u_1\|$. Then

$$(3) \lambda^{(n)}(\mu_1) = \mu_1 + \|Au_1 - \mu_1 u_1\| = \mu_1 + \sqrt{\|Au_1\|^2 - 2\mu_1(Au_1, u_1) + \mu_1^2}.$$

Let $f(\lambda)$ be defined by

$$(4) \quad f(\lambda) = \lambda + \sqrt{a - 2\lambda b + \lambda^2}, \quad \lambda \in (-\infty, +\infty)$$

where $a = \|A\mu_1\|^2$ and $b = (A\mu_1, \mu_1)$.

As $a \geq b^2$, the function $f(\lambda)$ is real and monotone increasing in $(-\infty, +\infty)$. Evidently, $\lambda^{(m)}(\mu_1) = f(\mu_1)$. Therefore, we find

$$(5) \quad f(\mu_0) \leq f(\mu_1) = \lambda^{(m)}(\mu_1).$$

Now, we note that

$$\|A\mu_1 - \mu_0 \mu_1\| \geq q_m(\mu_0)$$

and from (4) it follows

$$f(\mu_0) \geq \mu_0 + q_m(\mu_0) = \lambda^{(m)}(\mu_0)$$

so that $\lambda^{(m)}(\mu_0) \leq \lambda^{(m)}(\mu_1)$.

In the case $\mu_0 < \mu_1$, $\mu_0 \in I_2$ one finds similarly $\lambda^{(m)}(\mu_0) \leq \lambda^{(m)}(\mu_1)$.

An immediate consequence of Lemma 1 and Theorem 3 of [1] is the following

Theorem 1. Suppose an eigenvalue λ_j of A is not an accumulation point of $\sigma(A)$. Let $\mu_1, \mu_2, \mu_3, \mu_4$ be real numbers such that

$$\frac{1}{2}(\lambda_j + t_{j-1}) \leq \mu_1 < \mu_2 < \lambda_j < \mu_3 < \mu_4 \leq \frac{1}{2}(\lambda_j + t_{j+1})$$

where

$$t_{j-1} = \sup_{\substack{t \in \sigma(A) \\ t < \lambda_j}} t, \quad t_{j+1} = \inf_{\substack{t \in \sigma(A) \\ t > \lambda_j}} t.$$

Then

$$a) \quad \lambda_-^{(m)}(\lambda_j) \leq \lambda^{(m)}(\mu_3) \leq \lambda^{(m)}(\mu_4) \leq \lambda_j \leq \lambda^{(m)}(\mu_1) \leq \lambda^{(m)}(\mu_2) \leq \lambda_+^{(m)}(\lambda_j),$$

where

$$\lambda_{-}^{(m)}(\lambda_j) = \lambda_j - q_m(\lambda_j) ,$$

$$\lambda_{+}^{(m)}(\lambda_j) = \lambda_j + q_m(\lambda_j) ;$$

$$b) \lim_{m \rightarrow \infty} \lambda_{-}^{(m)}(\lambda_j) = \lim_{m \rightarrow \infty} \lambda_{+}^{(m)}(\lambda_j) = \lambda_j .$$

In words, this theorem says that the best upper approximation to λ_j is obtained when $\mu = \frac{1}{2}(\lambda_j + t_{j-1})$ and the best lower approximation when $\mu = \frac{1}{2}(\lambda_j + t_{j+1})$.

2. Let A be a DS-operator which is bounded below. Let $\lambda_1 < \lambda_2 < \lambda_3 < \dots$ be an enumeration of its distinct eigenvalues with an increasing order of values and μ be such a real number that $\mu < \lambda_1$. It follows from Theorem 1 that we shall obtain the best approximation to λ_1 from above when $\mu \rightarrow -\infty$. The next theorem gives an important information on the limit of the function $\lambda^{(m)}(\mu)$ when $\mu \rightarrow -\infty$.

Theorem 2. Let A be a DS-operator which is bounded below. Let λ_1 be the smallest eigenvalues of A . Then

$$(6) \quad \lim_{\mu \rightarrow -\infty} \lambda^{(m)}(\mu) = \min_{\substack{\mu \in \mathbb{R} \\ \mu \neq 0}} \frac{(A\mu, \mu)}{|\mu|^2} ,$$

where $\lambda^{(m)}(\mu)$ is the approximation to λ_1 .

Proof. Suppose that $\mu < \lambda_1$. Therefore, from (1) and (2) we see that

$$(7) \quad \lambda^{(n)}(\mu) = \mu + q_n(\mu) \leq \mu + \|A\mu - \mu\|$$

for each $\mu \in \mathcal{L}\{\psi_i\}_{i=1}^n$ such that $\|\mu\| = 1$.

Select $\mu \in \mathcal{L}\{\psi_i\}_{i=1}^n$, $\|\mu\| = 1$ and define $f(\lambda)$ by

$$(8) \quad f(\lambda) = \lambda + \sqrt{a - 2\lambda b + \lambda^2}$$

where $a = \|A\mu\|^2$ and $b = (A\mu, \mu)$.

It follows from (8) and (7) that

$$(9) \quad \lim_{\mu \rightarrow -\infty} \lambda^{(n)}(\mu) \leq \lim_{\mu \rightarrow -\infty} f(\mu).$$

It is easily verified that

$$(10) \quad \lim_{\mu \rightarrow -\infty} f(\mu) = (A\mu, \mu).$$

Since μ is an arbitrary element of $\mathcal{L}\{\psi_i\}_{i=1}^n$ such that $\|\mu\| = 1$, it follows from (9) and (10) that

$$(11) \quad \lim_{\mu \rightarrow -\infty} \lambda^{(n)}(\mu) \leq \min_{\substack{\mu \in \mathcal{L}\{\psi_i\}_{i=1}^n \\ \|\mu\|=1}} (A\mu, \mu).$$

By Theorem 4 of [1], we have

$$(12) \quad \lambda^{(n)}(\mu) = q_n(\mu) + \mu \geq \min_{\substack{\mu \in \mathcal{L}\{\psi_i\}_{i=1}^n \\ \|\mu\|=1}} (A\mu, \mu).$$

Therefore, by (9) and (10) we find

$$\lim_{\mu \rightarrow -\infty} \lambda^{(n)}(\mu) = \min_{\substack{\mu \in \mathcal{L}\{\psi_i\}_{i=1}^n \\ \|\mu\|=1}} (A\mu, \mu).$$

Remark 1. Under the assumptions of Theorem 2, let $\Lambda^{(n)}$ be the approximation to λ_1 obtained from applying the Ritz's method to the subspace $H_n = \mathcal{L}\{\psi_i\}_{i=1}^n$. By Theorem 4 of [1], we have

$$\Lambda^{(n)} = \min_{\substack{\mu \in H_n \\ \|\mu\|=1}} (A\mu, \mu)$$

and $\lambda_1 \leq \Lambda^{(n)} \leq \lambda^{(n)}(\mu)$ for every μ with $\mu \in H_n$.

From Theorem 2 we can deduce that the approximation to the smallest eigenvalue λ_1 by the Ritz's method is "a limit's case" of the approximations by the method of least squares, i.e., $\lim_{n \rightarrow \infty} \lambda^{(n)}(\mu) = \Lambda^{(n)}$ for any positive integer n .

3. In this section we shall consider the problem of approximating the eigenfunctions of DS-operator. Without loss of generality we may assume that $\mu = 0$. We shall suppose that the eigenvalues $\{\lambda_i\}_{i=1}^{\infty}$ of A satisfy the relations

$$(13) \quad 0 < |\lambda_1| < |\lambda_2| \leq |\lambda_3| \leq \dots$$

and λ_1 is a simple eigenvalue.

The following lemma is needed.

Lemma 2. With the assumption (13), let $\{v_n\}_{n=1}^{\infty}$ be a sequence of normalized functions belonging to $\mathcal{D}(A)$ such that $\lim_{n \rightarrow \infty} \|Av_n\| = |\lambda_1|$. Then there exists a convergent subsequence $\{v_{n_i}\}_{i=1}^{\infty}$ such that its limit is an eigenfunction of A belonging to λ_1 .

Proof. By Lemma 1 of [1]

$$v_n = \sum_{i=1}^{\infty} v_i^{(n)}, \quad \|Av_n\|^2 = \sum_{i=1}^{\infty} \lambda_i^2 \cdot \|v_i^{(n)}\|^2,$$

where $v_i^{(n)}$ is the projection of v_n on H_i and H_i is the closure of a linear manifold generated by the

eigenfunctions of A associated with the eigenvalue λ_2 .

Since v_n is a normalized function, we have

$$|Av_n|^2 - \lambda_1^2 = \sum_{i=2}^{\infty} (\lambda_i^2 - \lambda_1^2) \cdot \|v_i^{(n)}\|^2 \geq (\lambda_2^2 - \lambda_1^2) \cdot \sum_{i=2}^{\infty} \|v_i^{(n)}\|^2 \geq 0.$$

It follows that

$$(14) \quad \lim_{n \rightarrow \infty} \sum_{i=2}^{\infty} \|v_i^{(n)}\|^2 = 0$$

and

$$(15) \quad \lim_{n \rightarrow \infty} \|v_1^{(n)}\|^2 = 1.$$

Now, let φ_1 be an eigenfunction corresponding to the eigenvalue λ_1 such that $\|\varphi_1\| = 1$. Then $v_1^{(n)} = (v_n, \varphi_1)\varphi_1$ and from (15) it follows $\lim_{n \rightarrow \infty} |(v_n, \varphi_1)|^2 = 1$.

This implies that the sequence $\{v_n\}_{n=1}^{\infty}$ contains a subsequence $\{v_{n_k}\}_{k=1}^{\infty}$ such that

$$(16) \quad \lim_{k \rightarrow \infty} (v_{n_k}, \varphi_1) = e, \quad |e| = 1.$$

Now,

$$\|v_{n_k} - e\varphi_1\|^2 = \sum_{i=2}^{\infty} \|v_i^{(n_k)}\|^2 + [(v_{n_k}, \varphi_1) - e]^2.$$

Hence, by (15) and (16) the subsequence $\{v_{n_k}\}_{k=1}^{\infty}$ has the limit $e\varphi_1$ and the proof is completed.

Remark 2. In this argument we have assumed that the λ_1 is a simple eigenvalue of A . However, multiple eigenvalues do not give rise to any special difficulties.

Remark 3. Lemma 2 is not valid in the case when $\lambda_2 = -\lambda_1$. To prove this we denote φ_1, φ_2 the normalized eigenfunctions corresponding to λ_1, λ_2 , respectively. Now, let us make a special choice of v_n as

follows:

$$v_n = \frac{1}{\sqrt{2}} (\varphi_1 + \varphi_2), \quad n = 1, 2, \dots$$

Then $\|v_n\| = 1$ and $Av_n = \frac{1}{\sqrt{2}} \lambda_1 (\varphi_1 - \varphi_2)$,

whence $\|Av_n\| = |\lambda_1|$ and v_n is not an eigenfunction of A .

Corollary. Let u_n be a normalized function belonging to $\mathcal{L}\{\psi_i\}_{i=1}^n$ such that

$$\|Au_n\| = \min_{\substack{u \in \mathcal{L}\{\psi_i\}_{i=1}^n \\ \|u\|=1}} \|Au\|.$$

Under the hypotheses of Lemma 2 the sequence $\{u_n\}_{n=1}^{\infty}$ contains a convergent subsequence and every convergent subsequence has a limit normalized eigenfunction of A associated with the eigenvalue λ_1 . It follows that the sequence $\{u_n\}_{n=1}^{\infty}$ contains at most two accumulation points. These points are φ_1 and $-\varphi_1$, where φ_1 is a normalized eigenfunction of A associated with the eigenvalue λ_1 . If we assume that $\{u_n\}_{n=1}^{\infty}$ has one accumulation point, it follows from Lemma 2 that the sequence $\{u_n\}_{n=1}^{\infty}$ is converging.

The next theorem gives a useful information on the construction of the approximation of the eigenfunction φ_1 .

Theorem 3. Let A be a DS-operator and $\{\psi_i\}_{i=1}^{\infty}$ a totally complete system. Suppose the eigenvalues $\{\lambda_i\}_{i=1}^{\infty}$ of A satisfy the relations

$$0 < |\lambda_1| < |\lambda_2| \leq |\lambda_3| \leq \dots$$

and that the eigenvalue λ_1 is simple. Consider the

functions $u_n \in \mathcal{L}(\mathcal{V}_i)_{i=1}^m, n=1, 2, \dots$ with the following properties

- 1) $\|Au_n\| = \min_{\substack{u \in \mathcal{L}(\mathcal{V}_i)_{i=1}^m \\ \|u\|=1}} \|Au\|,$
- 2) $\|u_n\| = 1,$
- 3) $(u_n, u_{n+1}) \geq 0.$

Then the sequence $\{u_n\}_{n=1}^{\infty}$ converges to a normalized eigenfunction of A associated with the eigenvalue λ_1 .

Proof. To prove this theorem, assume the contrary. Let \mathcal{G}_1 be an eigenfunction of A corresponding to λ_1 such that $\|\mathcal{G}_1\| = 1$. Suppose that $\{u_n\}_{n=1}^{\infty}$ is not converging. Then by Corollary it follows that $\{u_n\}_{n=1}^{\infty}$ has two accumulation points \mathcal{G}_1 and $-\mathcal{G}_1$. Define the sets M, N as follows:

M consists of all u_n for which $(u_n, \mathcal{G}_1) \geq 0,$

N consists of all u_n for which $(u_n, \mathcal{G}_1) < 0.$

From Corollary it follows that M and N have the accumulation points \mathcal{G}_1 and $-\mathcal{G}_1$, respectively. Since $\{u_n\}_{n=1}^{\infty} = M \cup N$, there exists $u_m \in M$ and $u_{m+1} \in N$ such that

$$\|u_m - \mathcal{G}_1\| < \frac{1}{2}, \quad \|u_{m+1} + \mathcal{G}_1\| < \frac{1}{2}.$$

But

$$\begin{aligned} (u_m, u_{m+1}) &= (u_m - \mathcal{G}_1, u_{m+1}) + (\mathcal{G}_1, u_{m+1} + \mathcal{G}_1) - 1 \leq \\ &\leq \|u_m - \mathcal{G}_1\| + \|u_{m+1} + \mathcal{G}_1\| - 1 < 0 \end{aligned}$$

and this contradicts the assumption 3).

Remark 4. Theorem 3 is not true for the case

$$\lambda_2 = -\lambda_1.$$

Remark 5. In the case of the multiple eigenvalue λ_1 Theorem 3 is valid, if we assume that $(\mu_n, \mu_{n+1}) \geq \varepsilon > 0$ for $n = 1, 2, \dots$.

Remark 6. Let A be a DS-operator and let λ_{μ} be a simple eigenvalue of A . Suppose λ_{μ} is not an accumulation point of the spectrum $\sigma(A)$. Let μ be a real number such that

$$|\mu - \lambda_{\mu}| < \inf_{\substack{t \in \sigma(A) \\ t \neq \lambda_{\mu}}} |\mu - t|.$$

Then a convergence theorem similar to Theorem 3 can be established, if we apply Theorem 3 with $(A - \mu I)$ and $\lambda_j - \mu$ in place of A and λ_j , respectively.

Under the assumptions as in Theorem 3, we now study the problem of determining $\{\mu_n\}_{n=1}^{\infty}$. Without loss of generality we may assume that the system $\{\psi_i\}_{i=1}^{\infty}$ is orthonormal and $\mu_1 = \psi_1$.

Let q_m^2 be the smallest eigenvalue of the matrix $A_m = \{(A\psi_i, A\psi_j)\}_{i,j=1}^m$, i.e., $q_m^2 = \min_{\substack{\mu \in \mathbb{R} \\ \|\mu\|=1}} \|A\mu\|^2$.

To find $\mu_n = \sum_{i=1}^m \alpha_i \psi_i$, $n > 1$, we must determine the solution of the equations

$$(17) \quad \sum_{i=1}^m \alpha_i^{(n)} \cdot [(A\psi_j, A\psi_i) - \delta_{ij} q_m^2] = 0, \quad j = 1, \dots, m$$

for the m unknowns $\alpha_1^{(n)}, \dots, \alpha_m^{(n)}$ such that

$$(18) \quad \sum_{i=1}^m (\alpha_i^{(n)})^2 = 1$$

and

$$(19) \quad \sum_{i=1}^{m-1} \alpha_i^{(m)} \alpha_i^{(m-1)} \geq 0.$$

It is evident that the solution $\alpha^{(m)} = (\alpha_1^{(m)}, \dots, \alpha_m^{(m)})$ of (17) is an eigenvector of A_m corresponding to q_m^2 . If the rank of the matrix $B_m = A_m - q_m^2 \cdot I_m$ (I_m denotes the identity matrix) is equal to $m - 1$, it follows from (17), (18) and (19) that the conditions 1) - 3) of Theorem 3 determine a unique function u_m .

Now, we discuss the rank k_m of the matrix B_m . Let $k_m = m - k$ and let $\{\psi_{i=1}^{(j)}\}_{i=1}^{k_m}$, $\{\psi_{i=1}^{(j)}\}_{i=1}^k$ be an orthonormal basis for the space of the solutions of (17). Define V_k to be a k -dimensional space spanned by $\{\psi_{i=1}^{(j)}\}_{i=1}^k$ where $u_m^{(j)} = \sum_{i=1}^m \alpha_{ij}^{(m)} \cdot \psi_j$. Then we have

Lemma 3. Under the hypotheses as in Theorem 3, let the rank of the matrix B_m be equal to $m - k$, $1 \leq k \leq m$. Then

$$(Au, Av) = q_m^2 \cdot (u, v) \text{ for any } u, v \in V_k.$$

Proof. Let $q_m = \min_{\|u\|=1} \|Au\|$. Using the definition

of $u_m^{(i)}$, we have

$$(Au_m^{(i)}, A\psi_k) = \sum_{j=1}^m \alpha_{ji}^{(m)} \cdot (A\psi_j, A\psi_k) = q_m^2 \cdot \alpha_{ki}^{(m)}, \quad i = 1, \dots, k$$

and hence

$$(20) \quad (Au_m^{(i)}, A\psi_j) = \sum_{k=1}^k \alpha_{kj}^{(m)} q_m^2 \cdot \alpha_{ki}^{(m)} = q_m^2 \cdot \delta_{ij}.$$

Since $\{\mu_m^{(i)}\}_{i=1}^{\infty}$ is an orthonormal basis for $V_{\mathbb{R}}$, it follows from (20) that $(Au, Av) = \rho_m^2 \cdot (\mu, \nu)$ for any $\mu, \nu \in V_{\mathbb{R}}$. This proves the lemma.

As a consequence of Lemma 3, we have

Theorem 4. With the assumptions of Theorem 3, let the system $\{\Psi_i\}_{i=1}^{\infty}$ be orthonormal. Then there exists a positive integer n_0 such that the rank of the matrix $\beta_m = \{(A\Psi_i, A\Psi_j) - \alpha_{ij}^2 \cdot \rho_m^2\}_{i,j=1}^m$ is equal to $m-1$ for $m \geq n_0$, i.e., ρ_m^2 is a simple eigenvalue of the matrix $\beta_m = \{(A\Psi_i, A\Psi_j)\}_{i,j=1}^m$ for $m \geq n_0$.

Proof. Let us denote the rank of β_m by κ_m . Suppose that there exists an infinite set N of positive integers such that $\kappa_m < m-1$ for $m \in N$. Now, it follows from Lemma 3 that there exist μ_m, ν_m such that

$$1) \mu_m, \nu_m \in \mathcal{L}\{\Psi_i\}_{i=1}^m, \|\mu_m\| = \|\nu_m\| = 1,$$

$$(\mu_m, \nu_m) = (A\mu_m, A\nu_m)$$

$$2) \|A\mu_m\| = \|A\nu_m\| = \rho_m$$

for any $m \in N$. Consequently, $\lim_{\substack{m \rightarrow \infty \\ m \in N}} \|A\mu_m\| = \lim_{\substack{m \rightarrow \infty \\ m \in N}} \|A\nu_m\| = |\lambda_1|$.

It follows from Lemma 2 that we can choose convergent sequences $\{\nu_{m_i}\}_{i=1}^{\infty}$ and $\{\mu_{m_i}\}_{i=1}^{\infty}$ from $\{\mu_m\}_{m=1}^{\infty}$ and $\{\nu_m\}_{m=1}^{\infty}$ respectively, such that $\lim_{i \rightarrow \infty} \mu_{m_i} = \mu_0$

and $\lim_{i \rightarrow \infty} v_{m_i} = v_0$, where u_0 and v_0 are the normalized eigenfunctions corresponding to λ_1 . From this we obtain

$$(21) \quad (u_0, v_0) = 0.$$

On the other hand, λ_1 is a simple eigenvalue of A . Consequently, $|(u_0, v_0)| = 1$ and this contradicts (21).

Remark 7. With the assumptions of Theorem 3, the number q_n^2 is the smallest eigenvalue of the algebraic eigenvalue problem $(A_n - \sigma B_n)u = 0$, where

$$A_n = \{A\Psi_i, A\Psi_j\}_{i,j=1}^n \quad \text{and} \quad B_n = \{\Psi_i, \Psi_j\}_{i,j=1}^n$$

and there exists a positive integer n_0 such that the q_n^2 is simple for $n \geq n_0$. From this it follows that the conditions 1) - 3) of Theorem 3 determine a unique function u_n for $n \geq n_0$.

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