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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 axis and the spectrum $\sigma(A)$ is the closure of this set. Let λ_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

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

where

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

and λ_j is a fixed eigenvalue of A.
We remark that $\lim\limits_{n\to\infty} q_n=\inf\limits_{t\in\sigma(A)}|t-\mu|$ (Theorem 3 of [1],p.318). Before proving Theorem 1, we establish the following lemma.

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

<u>Proof</u>. 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 $q_n(\mu_1)=\|Au_1-\mu_1u_1\|$. Then

$$(3)\ \lambda^{(n)}(\mu_1)=\mu_1+\|Au_1-\mu_1u_1\|=\mu_1+\sqrt{\|Au_1\|^2-2\mu_1(Au_1,u_1)+\mu_1^2}.$$

Let $f(\lambda)$ be defined by

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

where $a=\|Au_1\|^2$ and $b=(Au_1,u_1)$.
As $a \geqslant b^2$, the function $f(\lambda)$ is real and monotone increasing in $(-\infty,+\infty)$. Evidently, $\lambda^{(n)}(\mu_1)=$ $=f(\mu_1)$. Therefore, we find

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

Now, we note that

$$\|Au_1-\mu_0 u_1\|\geq q_n(\mu_0)$$

and from (4) it follows

$$f(\mu_0)\geq\mu_0+q_n(\mu_0)=\lambda^{(n)}(\mu_0)$$

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

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

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 μ_1, μ_2, μ_3, μ_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) $$\lambda_-^{(n)}(\lambda_j)\leq\lambda^{(n)}(\mu_3)\leq\lambda^{(n)}(\mu_4)\leq\lambda_j\leq$$
$$\leq\lambda^{(n)}(\mu_1)\leq\lambda^{(n)}(\mu_2)\leq\lambda_+^{(n)}(\lambda_j)\,,$$

where

$$\lambda_-^{(n)}(\lambda_j) = \lambda_j - q_n(\lambda_j) \quad ,$$

$$\lambda_+^{(n)}(\lambda_j) = \lambda_j + q_n(\lambda_j) \quad ;$$

b) $\lim\limits_{n\to\infty} \lambda_-^{(n)}(\lambda_j) = \lim\limits_{n\to\infty} \lambda_+^{(n)}(\lambda_j) = \lambda_j$.

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 $\mu \to -\infty$. The next theorem gives an important information on the limit of the function $\lambda^{(n)}(\mu)$ when $\mu \to -\infty$.

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

(6) $$\lim_{\mu\to-\infty} \lambda^{(n)}(\mu) = \min_{\substack{u \in \mathcal{L}\{x_i\}_{i=1}^{n} \\ u \neq 0}} \frac{(Au, u)}{\|u\|^2} \quad ,$$

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

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

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

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

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

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

where $a = \|Au\|^2$ and $b = (Au, u)$.

It follows from (8) and (7) that

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

It is easily verified that

(10) $$\lim_{\mu\to-\infty} f(\mu) = (Au, u) .$$

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

(11) $$\lim_{\mu\to-\infty}\lambda^{(n)}(\mu) \leq \min_{\substack{u\in\mathcal{L}\{\Psi_i\}_{i=1}^{n}\\ \|u\|=1}} (Au, u) .$$

By Theorem 4 of [1], we have

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

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

$$\lim_{\mu\to-\infty}\lambda^{(n)}(\mu) = \min_{\substack{u\in\mathcal{L}\{\Psi_i\}_{i=1}^{n}\\ \|u\|=1}} (Au, u) .$$

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

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

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

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., $\lim_{\mu \to -\infty} \lambda^{(n)}(\mu) = \Lambda^{(n)}$ 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) $$0 < |\lambda_1| < |\lambda_2| \leq |\lambda_3| \leq \ldots$$

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 $\mathfrak{D}(A)$ such that $\lim_{n \to \infty} \|Av_n\| = |\lambda_1|$. 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_i. Since v_n is a normalized function, we have

$$\|Av_n\|^2-\lambda_1^2=\sum_{i=1}^{\infty}(\lambda_i^2-\lambda_1^2)\cdot\|v_i^{(n)}\|^2\geq(\lambda_2^2-\lambda_1^2)\cdot\sum_{i=2}^{\infty}\|v_i^{(n)}\|^2\geq 0 \ .$$

It follows that

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

and

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

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 $\lim_{n\to\infty}|(v_n,\varphi_1)|^2=1$.

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

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

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:

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

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.

<u>Corollary.</u> 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.

<u>Theorem 3</u>. 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

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

and that the eigenvalue λ_1 is simple. Consider the functions $u_n \in \mathcal{L}\{\psi_i\}_{i=1}^{n}, n=1,2,\ldots$ with the following properties

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

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 .

<u>Proof</u>. To prove this theorem, assume the contrary. Let φ_1 be an eigenfunction of A corresponding to λ_1 such that $\|\varphi_1\| = 1$. Suppose that $\{u_m\}_{m=1}^{\infty}$ is not converging. Then by Corollary it follows that $\{u_m\}_{m=1}^{\infty}$ has two accumulation points φ_1 and $-\varphi_1$. Define the sets M, N as follows:

M consists of all u_m for which $(u_m, \varphi_1) \geq 0$,

N consists of all u_m for which $(u_m, \varphi_1) < 0$.

From Corollary it follows that M and N have the accumulation points φ_1 and $-\varphi_1$, respectively. Since $\{u_n\}_{n=1}^{\infty} = M \cup N$, there exists $u_m \in M$ and $u_{m+1} \in N$ such that

$$\|u_m - \varphi_1\| < \frac{1}{2} , \quad \|u_{m+1} + \varphi_1\| < \frac{1}{2} .$$

But

$$(u_m, u_{m+1}) = (u_m - \varphi_1, u_{m+1}) + (\varphi_1, u_{m+1} + \varphi_1) - 1 \leq$$
$$\leq \|u_m - \varphi_1\| + \|u_{m+1} + \varphi_1\| - 1 < 0$$

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 $(u_n, u_{n+1}) \geq \geq \varepsilon > 0$ for $n = 1, 2, \dots$.

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

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

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 $\{u_n\}_{n=1}^{\infty}$. Without loss of generality we may assume that the system $\{\Psi_i\}_{i=1}^{\infty}$ is orthonormal and $u_1 = \Psi_1$.

Let q_n^2 be the smallest eigenvalue of the matrix $\mathcal{A}_n = \{(A\Psi_i, A\Psi_j)\}_{i,j=1}^{n}$, i.e., $q_n^2 = \min_{\substack{u \in \mathcal{L}\{\Psi_i\}_{i=1}^{n} \\ \|u\| = 1}} \|Au\|^2$.

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

$$(17) \quad \sum_{i=1}^{n} \alpha_i^{(n)} \cdot [(A\Psi_j, A\Psi_i) - \delta_{ij} q_n^2] = 0, \quad j = 1, \dots, n$$

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

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

and

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

It is evident that the solution $\alpha^{(n)} = (\alpha_1^{(n)}, \ldots, \alpha_n^{(n)})$ of (17) is an eigenvector of $\mathcal{A}_n$ corresponding to q_n^2. If the rank of the matrix $\mathcal{B}_n = \mathcal{A}_n - q_n^2 \cdot I_n$ (I_n denotes the identity matrix) is equal to $n-1$, it follows from (17),(18) and (19) that the conditions 1) - 3) of Theorem 3 determine a unique function u_n .

Now, we discuss the rank κ_n of the matrix $\mathcal{B}_n$. Let $\kappa_n = n - k$ and let $\{{}^{(j)}\alpha^{(n)}\}_{j=1}^{k}, {}^{(j)}\alpha^{(n)} = \{\alpha_{ij}^{(n)}\}_{i=1}^{n}$ be an orthonormal basis for the space of the solutions of (17). Define V_k to be a k-dimensional space spanned by $\{u_n^{(i)}\}_{i=1}^{k}$ where $u_n^{(i)} = \sum_{j=1}^{n} \alpha_{ij}^{(n)} \cdot \Psi_j$. Then we have

__Lemma 3.__ Under the hypotheses as in Theorem 3, let the rank of the matrix $\mathcal{B}_n$ be equal to $n-k$, $1 \leq k \leq n$. Then

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

__Proof__. Let $q_n = \min_{\substack{u \in \mathcal{L}\{\Psi_i\}_{i=1}^{n} \\ \|u\|=1}} \|Au\|$. Using the definition of $u_n^{(i)}$, we have

$$(Au_n^{(i)}, A\Psi_k) = \sum_{j=1}^{n} \alpha_{ji}^{(n)} \cdot (A\Psi_j, A\Psi_k) = q_n^2 \cdot \alpha_{ki}^{(n)}, \quad i = 1, \ldots, k$$

and hence

$$(20) \quad (Au_n^{(i)}, A_n^{(j)}) = \sum_{k=1}^{n} \alpha_{kj}^{(n)} q_n^2 \cdot \alpha_{ki}^{(n)} = q_n^2 \cdot \delta_{ij} \quad .$$

Since $\{u_n^{(i)}\}_{i=1}^{\infty}$ is an orthonormal basis for V_k, it follows from (20) that $(Au, Av) = q_n^2 \cdot (u, v)$ for any $u, v \in V_k$. This proves the lemma.

As a consequence of Lemma 3, we have

<u>Theorem 4</u>. 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 $\mathcal{B}_n = \{(A\Psi_i, A\Psi_j) - \delta_{ij} \cdot q_n^2\}_{i,j=1}^{n}$ is equal to $n-1$ for $n \geq n_0$, i.e., q_n^2 is a simple eigenvalue of the matrix $\mathcal{A}_n = \{(A\Psi_i, A\Psi_j)\}_{i,j=1}^{n}$ for $n \geq n_0$.

<u>Proof</u>. Let us denote the rank of $\mathcal{B}_n$ by κ_n. Suppose that there exists an infinite set N of positive integers such that $\kappa_n < n-1$ for $n \in N$. Now, it follows from Lemma 3 that there exist u_n, v_n such that

1) $u_n, v_n \in \mathcal{L}\{\Psi_i\}_{i=1}^{n}$, $\|u_n\| = \|v_n\| = 1$,
   $(u_n, v_n) = (Au_n, Av_n)$

2) $\|Au_n\| = \|Av_n\| = q_n$

for any $n \in N$. Consequently, $\lim\limits_{\substack{n\to\infty \\ n\in N}} \|Au_n\| = \lim\limits_{\substack{n\to\infty \\ n\in N}} \|Av_n\| = |\lambda_1|$.

It follows from Lemma 2 that we can choose convergent sequences $\{v_{n_i}\}_{i=1}^{\infty}$ and $\{u_{n_i}\}_{i=1}^{\infty}$ from $\{u_n\}_{\substack{n=1 \\ n\in N}}^{\infty}$ and $\{v_n\}_{\substack{n=1 \\ n\in N}}^{\infty}$, respectively, such that $\lim\limits_{i\to\infty} u_{n_i} = u_0$

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

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

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_m^2 is the smallest eigenvalue of the algebraic eigenvalue problem $(\mathcal{A}_m - \sigma \mathcal{B}_m) u = 0$, where $\mathcal{A}_m = \{(A\Psi_i, A\Psi_j)\}_{i,j=1}^{m}$ and $\mathcal{B}_m = \{(\Psi_i, \Psi_j)\}_{i,j=1}^{m}$ and there exists a positive integer m_0 such that the q_m^2 is simple for $m \geq m_0$. From this it follows that the conditions 1) - 3) of Theorem 3 determine a unique function u_m for $m \geq m_0$.

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