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

K. NAJZAR, Praha

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 $\lambda$ depends on a parameter $\mu$, i.e., $\lambda^{(n)} = \lambda^{(n)}(\mu)$ and we can obtain upper or lower bounds of $\lambda$ for appropriate choice of $\mu$. In this paper, we shall consider the problem of the optimum choice of the $\mu$ which leads to an error $\lambda^{(m)}(\mu) - \lambda$ 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 $\lambda_i$, $i = 1, 2, \ldots$ be an enumeration of distinct eigenvalues of $A$. Further, we assume that $\{\lambda_i\}_{i=1}^{\infty}$ is a totally complete system.

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

\begin{align*}
(1) \quad \lambda^{(m)}(\mu) &= \begin{cases} 
\mu + q_m(\mu) & \text{for } \mu < \lambda_j, \\
\mu - q_m(\mu) & \text{for } \mu > \lambda_j,
\end{cases}
\end{align*}

where

\begin{equation}
q_m(\mu) = \min_{\|u\| = 1} \frac{||Au - \mu u||}{\|u\|}
\end{equation}

and $\lambda_j$ is a fixed eigenvalue of $A$.

We remark that $\lim_{m \to \infty} q_m = \inf_{t \in \sigma(A)} |t - \mu|$ (Theorem 3 of [11, p.318]). Before proving Theorem 1, we establish the following lemma.

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

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

\begin{equation}
(3) \quad \lambda^{(m)}(\mu_0) = \mu_0 + ||Au_1 - \mu_0 u_1|| = \mu_0 + \sqrt{||Au_1||^2 - 2\mu_0 (Au_1, u_1) + \mu_0^2}.
\end{equation}

Let $f(\lambda)$ be defined by
where $\lambda = \|A\mu_1\|_2$ 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

\begin{align*}
(5) \quad f(\mu_0) \leq f(\mu_1) = \lambda^{(m)}(\mu_1) .
\end{align*}

Now, we note that

\begin{align*}
\|A\mu_1 - \mu_0 \mu_1\| \geq \varphi_m(\mu_0)
\end{align*}

and from (4) it follows

\begin{align*}
f(\mu_0) \geq (\mu_0 + \varphi_m(\mu_0)) = \lambda^{(m)}(\mu_0)
\end{align*}

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

\begin{align*}
\lambda^{(m)}(\mu_0) \leq \lambda^{(m)}(\mu_1) .
\end{align*}

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

**Theorem 1.** Suppose an eigenvalue $\lambda_1$ of $A$ is not an accumulation point of $\sigma(A)$. Let $\mu_1$, $\mu_2$, $\mu_3$, $\mu_4$ be real numbers such that

\begin{align*}
\frac{1}{2}(\lambda_1 + t_{j-1}) < \mu_1 < \mu_2 < \lambda_j < \mu_3 < \mu_4 \leq \frac{1}{2}(\lambda_j + t_{j+1})
\end{align*}

where

\begin{align*}
t_{j-1} = \sup_{t \in \sigma(A)} t, \quad t_{j+1} = \inf_{t \in \sigma(A)} t .
\end{align*}

Then

\begin{align*}
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) ,
\end{align*}

where
\[ \lambda^{(m)}_-(\lambda_j) = \lambda_j - q_n(\lambda_j), \]
\[ \lambda^{(m)}_+(\lambda_j) = \lambda_j + q_n(\lambda_j), \]

b) \[ \lim_{n \to \infty} \lambda^{(m)}_-(\lambda_j) = \lim_{n \to \infty} \lambda^{(m)}_+(\lambda_j) = \lambda_j. \]

In words, this theorem says that the best upper approximation to \( \lambda_j \) 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 \( \lambda_1 < \lambda_2 < \lambda_3 < \ldots \) be an enumeration of its distinct eigenvalues with an increasing order of values and \( \mu \) be such a real number that \( \mu < \lambda_1 \). It follows from Theorem 1 that we shall obtain the best approximation to \( \lambda_j \) from above when \( \mu \to -\infty \). The next theorem gives an important information on the limit of the function \( \lambda^{(m)}(\mu) \) when \( \mu \to -\infty \).

**Theorem 2.** Let \( A \) be a DS-operator which is bounded below. Let \( \lambda_1 \) be the smallest eigenvalues of \( A \). Then

\[ \lim_{\mu \to -\infty} \lambda^{(m)}(\mu) = \min_{\mu \neq \lambda_1} \frac{(A\mu, \mu)}{1|\mu|^2}, \]

where \( \lambda^{(m)}(\mu) \) is the approximation to \( \lambda_1 \).

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

\[
f(\lambda) = \lambda + \sqrt{a - 2\lambda \nu + \lambda^2}
\]

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

It follows from (8) and (7) that

\[
\lim_{\mu \to -\infty} \lambda^{m,\mu}(u) \leq \lim_{\mu \to -\infty} f(\mu).
\]

It is easily verified that

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

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

\[
\lim_{\mu \to -\infty} \lambda^{m,\mu}(u) \leq \min_{||u|| = 1} (Au, u).
\]

By Theorem 4 of [1], we have

\[
\lambda^{m,\mu}(u) = q_{m,\mu}(u) + \mu \geq \min_{||u|| = 1} (Au, u).
\]

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

\[
\lim_{\mu \to -\infty} \lambda^{m,\mu}(u) = \min_{||u|| = 1} (Au, u)
\]

Remark 1. Under the assumptions of Theorem 2, let \( \lambda^{(n)} \) be the approximation to \( \lambda \) 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
\[ \lambda^{(m)} = \min_{\mu \in \mathbb{C}, \|\mu\| = 1} (A\mu, \mu) \]

and \( \lambda_1 \leq \lambda^{(m)} \leq \lambda^{(m)}(\mu) \) for every \( \mu \) with \( \mu \leq \lambda_q \).

From Theorem 2 we can deduce that the approximation to the smallest eigenvalue \( \lambda_q \) by the Ritz's method is "a limit's case" of the approximations by the method of least squares, i.e.,

\[ \lim_{\mu \to \infty} \lambda^{(m)}(\mu) = \lambda^{(m)} \]

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

\[ 0 < |\lambda_1| < |\lambda_2| \leq |\lambda_3| \leq \ldots \]

and \( \lambda_q \) 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 \( \lim_{n \to \infty} \|A v_n\| = |\lambda_q| \). Then there exists a convergent subsequence \( \{v_{n_k}\}_{k=1}^{\infty} \) such that its limit is an eigenfunction of \( A \) belonging to \( \lambda_q \).

**Proof.** By Lemma 1 of [1]

\[ v_n = \frac{v_{n}^{(m)}}{\|v_{n}^{(m)}\|}, \quad \|A v_n\|^2 = \sum_{i=1}^{m} \lambda_i^2 \cdot |v_{n}^{(m)}i|^2, \]

where \( v_{n}^{(m)} \) is the projection of \( v_n \) on \( \mathcal{H}_n \) and \( \mathcal{H}_n \) is the closure of a linear manifold generated by the
eigenfunctions of $A$ associated with the eigenvalue $\lambda_i$. Since $\nu_m$ is a normalized function, we have

$$|A
\nu_m|^2 - \lambda_i^2 = \sum_{i=2}^\infty (\lambda_i^2 - \lambda_i^2) \cdot \|\nu_m^{(m)}\|^2 \geq (\lambda_2^2 - \lambda_1^2) \cdot \sum_{i=2}^\infty \|\nu_i^{(m)}\|^2 \geq 0.$$ 

It follows that

$$\lim_{n \to \infty} \sum_{i=2}^\infty \|\nu_i^{(m)}\|^2 = 0 \quad \text{(14)}$$

and

$$\lim_{n \to \infty} \|\nu_i^{(m)}\|^2 = 1 \quad \text{(15)}$$

Now, let $\varphi_i$ be an eigenfunction corresponding to the eigenvalue $\lambda_i$ such that $\|\varphi_i\| = 1$. Then $\nu_i^{(m)} = (\nu_m, \varphi_i) \varphi_i$ and from (15) it follows $\lim_{n \to \infty} |(\nu_m, \varphi_i)|^2 = 1$.

This implies that the sequence $\{\nu_m^{(m)}\}_{m=1}^{\infty}$ contains a subsequence $\{\nu_m^{(m)}\}_{m=1}^{\infty}$ such that

$$\lim_{n \to \infty} (\nu_m, \varphi_i) = e, \quad |e| = 1 \quad \text{(16)}$$

Now,

$$|\nu_m^{(m)} - e \varphi_i|^2 = \sum_{i=2}^\infty \|\nu_i^{(m)}\|^2 + |(\nu_m^{(m)}, \varphi_i) - e|^2.$$ 

Hence, by (15) and (16) the subsequence $\{\nu_m^{(m)}\}_{m=1}^{\infty}$ has the limit $e \varphi_i$ and the proof is completed.

**Remark 2.** In this argument we have assumed that the $\lambda_i$ 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 $\varphi_1$, $\varphi_2$ the normalized eigenfunctions corresponding to $\lambda_1$, $\lambda_2$, respectively. Now, let us make a special choice of $\nu_m$ as
follows:
\[ v_n = \frac{1}{\sqrt{2}} (\varphi_1 + \varphi_2), \quad n = 1, 2, \ldots \]
Then \( |v_n| = 1 \) and \( A v_n = \frac{1}{\sqrt{2}} \lambda_n (\varphi_1 - \varphi_2) \),
whence \( |A v_n| = |\lambda_n| \) and \( v_n \) is not an eigenfunction of \( A \).

Corollary. Let \( \mu_n \) be a normalized function belonging to \( L^2 \left[ a, b \right] \) such that
\[ |A \mu_n| = \min_{\mu \in L^2 \left[ a, b \right]} ||A \mu||. \]
Under the hypotheses of Lemma 2 the sequence \( \{\mu_n\}_{n=1}^{\infty} \) contains a convergent subsequence and every convergent subsequence has a limit normalized eigenfunction of \( A \) associated with the eigenvalue \( \lambda_n \). It follows that the sequence \( \{\mu_n\}_{n=1}^{\infty} \) contains at most two accumulation points. These points are \( \varphi_1 \) and \( -\varphi_1 \), where \( \varphi_1 \) is a normalized eigenfunction of \( A \) associated with the eigenvalue \( \lambda_1 \). If we assume that \( \{\mu_n\}_{n=1}^{\infty} \) has one accumulation point, it follows from Lemma 2 that the sequence \( \{\mu_n\}_{n=1}^{\infty} \) is converging.

The next theorem gives a useful information on the construction of the approximation of the eigenfunction \( \varphi_1 \).

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
\[ 0 < |\lambda_1| < |\lambda_2| \leq |\lambda_3| \leq \ldots \]
and that the eigenvalue \( \lambda_1 \) is simple. Consider the
functions $\mu_m \in L^2_{\int_{t_0}^{t_1} d t}, m = 1, 2, \ldots$ with the following properties

1) $\| A \mu_m \| = \min_{\mu \in L^2_{\int_{t_0}^{t_1} d t}} \| A \mu \|,$

2) $\| \mu_m \| = 1,$

3) $(\mu_m, \mu_{m+1}) \geq 0.$

Then the sequence $\{\mu_m\}_{m=1}^{\infty}$ converges to a normalized eigenfunction of $A$ associated with the eigenvalue $\lambda_1$.

**Proof.** To prove this theorem, assume the contrary. Let $\varphi_1$ be an eigenfunction of $A$ corresponding to $\lambda_1$ such that $\| \varphi_1 \| = 1$. Suppose that $\{\mu_m\}_{m=1}^{\infty}$ is not converging. Then by Corollary it follows that $\{\mu_m\}_{m=1}^{\infty}$ has two accumulation points $\varphi_1$ and $-\varphi_1$.

Define the sets $M, N$ as follows:

- $M$ consists of all $\mu_m$ for which $(\mu_m, \varphi_1) \geq 0,$
- $N$ consists of all $\mu_m$ for which $(\mu_m, \varphi_1) < 0.$

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

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

But

$$(\mu_m, \mu_{m+1}) = (\mu_m - \varphi_1, \mu_{m+1}) + (\varphi_1, \mu_{m+1} + \varphi_1) - 1 \leq$$

$$\leq \| \mu_{m} - \varphi_1 \| + \| \mu_{m+1} + \varphi_1 \| - 1 < 0$$

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 \( \lambda_1 \), Theorem 3 is valid, if we assume that \((\omega_m, \omega_{m+1}) \geq \varepsilon > 0 \) for \( m = 1, 2, \ldots \).

Remark 6. Let \( A \) be a DG-operator and let \( \lambda_{\text{sc}} \) be a simple eigenvalue of \( A \). Suppose \( \lambda_{\text{sc}} \) is not an accumulation point of the spectrum \( \sigma(A) \). Let \( \mu \) be a real number such that
\[ |\mu - \lambda_{\text{sc}}| < \inf_{t \in \sigma(A)} |\mu - t|. \]
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 \( \lambda_j \), respectively.

Under the assumptions as in Theorem 3, we now study the problem of determining \( \{\omega_m\}_{m=1}^{\infty} \). Without loss of generality we may assume that the system \( \{\Psi_i\}_{i=1}^{\infty} \) is orthonormal and \( \omega_1 = \Psi_1 \).

Let \( q_m^2 \) be the smallest eigenvalue of the matrix \( \lambda_m = \{(A\Psi_i, A\Psi_j)\}_{i,j=1}^{\infty} \), i.e., \( q_m^2 = \min_{\lambda_m \in \sigma(A)} \|A\mu\|^2 \).
To find \( \omega_m = \sum_{i=1}^{\infty} \alpha_i^{(m)} \Psi_i \), \( m > 1 \), we must determine the solution of the equations
\[ \sum_{i=1}^{\infty} \alpha_i^{(m)} [(A\Psi_i, A\Psi_j) - \delta_{ij} q_m^2] = 0, \quad j = 1, \ldots, n \]
for the \( m \) unknowns \( \alpha_1^{(m)}, \ldots, \alpha_n^{(m)} \) such that
\[ \sum_{i=1}^{n} (\alpha_i^{(m)})^2 = 1. \]
and

$$(19) \sum_{i=1}^{n-1} \alpha_i^{(m)} \sigma_i^{(m-1)} \geq 0.$$ \hspace{1em}

It is evident that the solution $\alpha^{(m)} = (\alpha_1^{(m)}, \ldots, \alpha_n^{(m)})$ of (17) is an eigenvector of $A_m$ corresponding to $q_m^2$.

If the rank of the matrix $B_m = A_m - q_m^2 \cdot I_m$ (where $I_m$ 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 $\mu_m$.

Now, we discuss the rank $\kappa_m$ of the matrix $B_m$.

Let $\kappa_m = n - \kappa$ and let $\{\varphi^{(m)}_{\kappa}, \varphi^{(m)}_{\kappa+1}, \ldots, \varphi^{(m)}_n\}$ be an orthonormal basis for the space of the solutions of (17). Define $V_{\kappa}$ to be a $\kappa$-dimensional space spanned by $\{\varphi^{(m)}_i\}_{i=1}^{\kappa}$, where $\varphi^{(m)}_i = \frac{1}{\sqrt{2}} \varphi^{(m)}_{\kappa+i}$. Then we have

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

$$(A\mu, A\nu) = q_m^2 \cdot (\mu, \nu)$$

for any $\mu, \nu \in V_{\kappa}$.

**Proof.** Let $q_m = \min_{\mu \in V_{\kappa}} \|A\mu\|$. Using the definition of $q^{(m)}$, we have

$$\frac{1}{2} A\mu^{(m)} = \frac{1}{2} q_m \varphi^{(m)}_i, \quad \frac{1}{2} A\nu^{(m)} = \frac{1}{2} q_m \varphi^{(m)}_i, \quad i = 1, \ldots, \kappa$$

and hence

$$(20) (A\mu^{(m)}, A\nu^{(m)}) = \sum_{\kappa=1}^{\kappa} \alpha^{(m)}_i q_m^2, \quad \alpha^{(m)}_i = q_m \cdot \sigma_i.$$
Since \( \{ \mu^n_m \}_{i=1}^{\infty} \) is an orthonormal basis for \( V_k \), it follows from (20) that \( (A\mu, A\nu) = q^n\mu, (\mu, \nu) \) for any \( \mu, \nu \in V_k \). This proves the lemma.

As a consequence of Lemma 3, we have

**Theorem 4.** With the assumptions of Theorem 3, let the system \( \{ \gamma_i \}_{i=1}^{\infty} \) be orthonormal. Then there exists a positive integer \( n_0 \) such that the rank of the matrix \( B_m = \{ (A\gamma_i, A\gamma_j) - q^{-1} \gamma_i, \gamma_j \}_{i=1}^{\infty} \) is equal to \( n - 1 \) for \( m > n_0 \), i.e., \( q^2 \) is a simple eigenvalue of the matrix \( B_m = \{ (A\gamma_i, A\gamma_j) \}_{i=1}^{m} \) for \( m > n_0 \).

**Proof.** Let us denote the rank of \( B_m \) by \( \kappa_m \). Suppose that there exists an infinite set \( N \) of positive integers such that \( \kappa_m < n - 1 \) for \( m \in N \).

Now, it follows from Lemma 3 that there exist \( \mu_m, \nu_m \) such that

1) \( \mu_m, \nu_m \in \{ \gamma_i \}_{i=1}^{\infty}, \| \mu_m \| = \| \nu_m \| = 1 \),

\[ (\mu_m, \nu_m) = (A\mu_m, A\nu_m) \]

2) \( \| A\mu_m \| = \| A\nu_m \| = q^n \)

for any \( m \in N \). Consequently, \( \lim_{m \to \infty} \| A\mu_m \| = \lim_{m \to \infty} \| A\nu_m \| = |\lambda_1| \).

It follows from Lemma 2 that we can choose convergent sequences \( \{ \mu^n_i \}_{i=1}^{\infty} \) and \( \{ \mu^n_i \}_{i=1}^{\infty} \) from \( \{ \mu^n_m \}_{m=1}^{\infty} \) and \( \{ \nu^n_m \}_{m=1}^{\infty} \), respectively, such that \( \lim_{m \to \infty} \mu^n_m = \mu \).
and \( \lim_{i \to \infty} v_{n_i} = v_0 \), where \( u_0 \) and \( v_0 \) are the normalized eigenfunctions corresponding to \( \lambda_1 \). From this we obtain

\[(21) \quad (u_0, v_0) = 0.\]

On the other hand, \( \lambda_1 \) 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 \( q_{n_0}^2 \) is the smallest eigenvalue of the algebraic eigenvalue problem \((A_m - \theta B_m)u = 0\), where

\[
A_m = \{ (A\xi_i, A\xi_j) \}_{i,j=1}^{n} \quad \text{and} \quad B_m = \{ (\xi_i, \xi_j) \}_{i,j=1}^{n},
\]

and there exists a positive integer \( m_0 \) such that the \( q_{n_0}^2 \) is simple for \( n \geq m_0 \). From this it follows that the conditions 1) - 3) of Theorem 3 determine a unique function \( u_m \) for \( n \geq m_0 \).

**References**


Matematicko-fyzikální fakulta
Karlová universita
Malostranské nám.25
Praha 1, Československo

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