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TWO STEP EXTRAPOLATION AND OPTIMUM CHOICE OF RELAXATION FACTOR OF THE EXTRAPOLATED S.O.R. METHOD

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Summary. Limits of the extrapolation coefficients are rational functions of several poles with the largest moduli of the resolvent operator $R(\lambda, T) = (\lambda I - T)^{-1}$ and therefore good estimates of these poles could be calculated from these coefficients. The calculation is very easy for the case of two coefficients and its practical effect in finite dimensional space is considerable. The results are used for acceleration of S.O.R. method.

Keywords: Iterative process, extrapolation, S.O.R. method

AMS Classification: 65F10, 65B05

1. INTRODUCTION

In the paper [1] a possibility of improving the convergence of a sequence $\{x_j\}_{j=0}^{\infty}$ which is obtained from a convergent iterative process

$$x_{j+1} = Tx_j + b \tag{1.1}$$

for solving an operator equation

$$x = Tx + b \tag{2.1}$$

in a Hilbert space X was investigated. The symbol T will always denote a linear bounded operator on X with spectral radius $r(T) < 1$. Therefore for every $x_0 \in X$ the sequence $\{x_j\}_{j=0}^{\infty}$ obtained by using (1.1) is convergent with a limit $x^* = Tx^* + b$. The scalar product in X will be denoted by $(\cdot, \cdot)$ and the norm $\|x\| = (x, x)^{1/2}$ for every $x \in X$. Let $l > 0$, $k, m_0, m_1, \ldots, m_l$ be integers such that the inequalities

$$k > m_l > m_{l-1} > \ldots > m_1 > m_0 = 0 \tag{3.1}$$

hold. For a given positive integer n let $H = I - T^n$. Moreover, we define the norm $\|x\|_H = \|Hx\|$ for all x.

The principal idea given in [1] for improving the convergence consists in the construction of new approximations

$$y_k = \alpha_0^{(k)} x_k + \alpha_1^{(k)} x_{k-m_1} + \ldots + \alpha_l^{(k)} x_{k-m_l}$$

to x^*, where the condition for the complex numbers $\alpha_i^{(k)}$ is

$$\|x^* - \sum_{i=0}^{l} \alpha_i^{(k)} x_{k-m_i}\|_H = \min_{\substack{\beta_0+\ldots+\beta_l=1 \\ \beta_i \in C}} \|x^* - \sum_{i=0}^{l} \beta_i x_{k-m_i}\|_H , \tag{4.1}$$

$$\sum_{i=0}^{l} \alpha_i^{(k)} = 1 . \tag{4.1'}$$

This construction of a new sequence $\{y_k\}$ will be called an extrapolation and the numbers $\alpha_i^{(k)}$ the coefficients of extrapolation.

We put

$$\varepsilon_k = x^* - x_k ; \quad \eta_k = (I - T^n)\, \varepsilon_k , \tag{5.1}$$

$$\mathbf{Q}_k = \begin{pmatrix} (\eta_k, \eta_k), & (\eta_{k-m_1}, \eta_k), & (\eta_{k-m_2}, \eta_k), \ldots, & (\eta_{k-m_l}, \eta_k) \\ (\eta_k, \eta_{k-m_1}), & (\eta_{k-m_1}, \eta_{k-m_1}), & (\eta_{k-m_2}, \eta_{k-m_1}), \ldots, & (\eta_{k-m_l}, \eta_{k-m_1}) \\ \ldots & \ldots & \ldots & \ldots \\ (\eta_k, \eta_{k-m_l}), & (\eta_{k-m_1}, \eta_{k-m_l}), & (\eta_{k-m_2}, \eta_{k-m_l}), \ldots, & (\eta_{k-m_l}, \eta_{k-m_l}) \end{pmatrix} \tag{6.1}$$

and

$$\boldsymbol{\alpha}^{(k)} = (\alpha_0^{(k)}, \alpha_1^{(k)}, \ldots, \alpha_l^{(k)})^{\mathrm{T}} . \tag{7.1}$$

It is easy to see from (5.1) that

$$\eta_k = x_{k+n} - x_k . \tag{8.1}$$

We have proved in [1] that if the matrix $\mathbf{Q}_k$ is positive definite then there exists one and only one vector $\boldsymbol{\alpha}^{(k)} = (\alpha_0^{(k)}, \alpha_1^{(k)}, \ldots, \alpha_l^{(k)})^{\mathrm{T}}$ which solves the problem (4.1), (4.1'). It was shown that

$$\boldsymbol{\alpha}^{(k)} = (\mathbf{e}^{\mathrm{T}} \mathbf{Q}_k \mathbf{e})^{-1}\, \mathbf{Q}_k^{-1} \mathbf{e}, \text{ where } \mathbf{e} = (1, 1, \ldots, 1)^{\mathrm{T}}. \tag{9.1}$$

Moreover, we have proved in [2] that there exists $p \geqq 1$ such that

$$\lim_{k \to \infty} (\|x^* - y_k\| / \|x^* - x_k\|^p) = 0 ,$$

and in the same paper convergence and limits of $\alpha_i^{(k)}$ were studied. Limits of the extrapolation coefficients are rational functions of several poles with the largest moduli of the resolvent operator $R(\lambda, T) = (\lambda T - T)^{-1}$, and therefore good estimations of these poles could be calculated from $\alpha_i^{(k)}$. The calculation is, indeed, easy for $l = 1$ and its practical effect in a finite dimensional space is considerable.

Let us consider a system of linear algebraic equations

$$Ax = b , \tag{10.1}$$

with a positive definite $t \times t$ matrix A. Let $A = D - E - F$ where D is the diagonal of A, while E and F are strictly lower and upper triangular $t \times t$ matrices, respectively. The successive overrelaxation iterative method (S.O.R. method) applied to (10.1) gives for $\omega \in (0, 2)$ the convergent iterative process

$$(11.1) \qquad x_{j+1}(\omega) = \mathscr{L}_\omega x_j(\omega) + c(\omega)\,, \quad \text{where}$$

$$\mathscr{L}_\omega = (D - \omega E)^{-1} (\omega F + (1 - \omega) D) \quad \text{and} \quad c(\omega) = \omega(D - \omega E)^{-1} b\,.$$

If A has property **A**, the optimal choice of ω is given by $\omega_1 = 2/(1 + \sqrt{(1 - \mu_1^2)})$, where μ_1 is the spectral radius of the Jacobi matrix $D^{-1}(E + F)$. Let us put $y_k(\omega) = \alpha_0^{(k)} x_k(\omega) + \alpha_1^{(k)} x_{k-n}(\omega)$, where $k \geqq n$ is an integer. We shall see later that the optimal ω_2 which minimizes the R_1-factor (i.e. the number $\limsup_{k\to\infty} \|\mathbf{x}^* - \mathbf{y}_k(\omega)\|^{1/k}$) is given by $\omega_2 = 2/(1 + \sqrt{(1 - \mu_2^2)})$, where $\mu_1 > \mu_2 > \ldots > \mu_s > 0$ are all positive and mutually different eigenvalues of the Jacobi matrix. This is not convenient for the practical use. Nevertheless, the investigation given in this paper leads to an algorithm which gives very good estimates for ω_2 without any knowledge of the eigenvalues μ_i. Moreover, these estimates are calculated simultaneously with the iterations and require only a little more work. Numerical examples show the effectivity of this process in comparison with the optimal S.O.R..

The paper is organized in several parts. First, we present the theoretical investigation from which the behaviour of $\alpha_0^{(k)}$, $\alpha_1^{(k)}$ and y_k as functions of k follows. Then we calculate the first two poles of $R(\lambda, T)$. Application to S.O.R. method and numericcal results of a model example from reactor engineering conclude the paper.

2. AUXILIARY THEOREMS

Let the symbol C denote the set of complex numbers. Let the spectrum of T have the following structure: There exist finite sequences $\{i_k\}_{k=1}^r$ of positive integers and $\{\lambda_k\}_{k=1}^r \subset C$ for some integer $r > 2$ such that each λ_k is a pole of the resolvent operator of the order i_k,

$$(1.2) \qquad \lambda_1 = |\lambda_1| > |\lambda_2| > |\lambda_3| \geqq |\lambda_4| \geqq \ldots \geqq |\lambda_r|\,,$$

$$(2.2) \qquad \lambda_i \neq \lambda_j \quad \text{for} \quad i \neq j\,, \quad \text{and}$$

$$(3.2) \qquad \{\lambda \in \sigma(T), \lambda \neq \lambda_i,\ i = 1, \ldots, r\} \Rightarrow |\lambda| < |\lambda_r|\,.$$

For a fixed $j \in \langle 1, r\rangle$ let C_j be the circumference with center λ_j and radius $\varrho_j > 0$ such that

$$\{\lambda \in C \mid |\lambda - \lambda_j| \leqq \varrho_j\} \cap \sigma(T) = \{\lambda_j\}\,.$$

Let $K = \{\lambda \in C \mid |\lambda| = \tau\}$, where $\tau > r(T)$ and $C_0 = \{\lambda \in C \mid |\lambda| = \varrho_0\}$, where ϱ_0 is taken such that

$$\{\lambda \in C \mid |\lambda| \leqq \varrho_0\} \cap \sigma(T) = \sigma(T) \dot{-} \{\lambda_1, \ldots, \lambda_r\}\,.$$

We will assume without any loss of generality that

$$(4.2) \qquad B_{ji_j}\varepsilon_0 \neq 0 \quad \text{for all} \quad j = 1, 2, \ldots, r\,,$$

where

$$B_{ji} = \frac{1}{2\pi i} \int_{C_j} (\lambda - \lambda_j)^{i-1} R(\lambda, T) \, d\lambda$$

for all $j = 1, 2, \ldots, r$, and for every j we have $i = 1, 2, \ldots, i_j$.

Assumption 1. *Let*

(5.2) $$l = 1, \quad i_1 = 1,$$

(6.2) $$m_1 < \sum_{j=1}^{r} i_j, \quad i_3 = \max \{ i_s \mid |\lambda_3| = |\lambda_s| \}. \qquad \square$$

Put

(7.2) $$n = m_1 \quad \text{and} \quad k_0 = \max (i_j) + n.$$

Let us denote

(8.2) $$v_{ji} = (I - T^n) B_{ji} \varepsilon_0 / \lambda_j^{i-1}.$$

Lemma 1.2. *The equality*

(9.2) $$\eta_k = \sum_{j=1}^{r} \sum_{i=1}^{i_j} \binom{k}{i-1} \lambda_j^k v_{ji} + v(k)$$

holds for $k > k_0$, *where*

(10.2) $$v(k) = (I - T^n) \left(\frac{1}{2\pi i} \int_{C_0} \lambda^k R(\lambda, T) \, \varepsilon_0 \, d\lambda \right).$$

All vectors v_{ji} *are linearly independent.*

Proof. We have

$$\varepsilon_k = T^k \varepsilon_0 = \frac{1}{2\pi i} \int_K \lambda^k R(\lambda, T) \, \varepsilon_0 \, d\lambda =$$

$$= \sum_{j=1}^{r} \frac{1}{2\pi i} \int_{C_j} \lambda^k R(\lambda, T) \, \varepsilon_0 \, d\lambda + \frac{1}{2\pi i} \int_{C_0} \lambda^k R(\lambda, T) \, \varepsilon_0 \, d\lambda =$$

$$= \sum_{j=1}^{r} \sum_{i=1}^{i_j} \binom{k}{i-1} \lambda_j^{k-i+1} B_{ji} \varepsilon_0 + \frac{1}{2\pi i} \int_{C_0} \lambda^k R(\lambda, T) \, \varepsilon_0 \, d\lambda.$$

From (8.2) the equalities (9.2) and (10.2) immediately follow. In order to prove the second statement of this lemma, it suffices to prove that the vectors $B_{ji}\varepsilon_0$ are linearly independent. But this immediately follows by virtue of the relations $B_{j,i_j+1} = 0$ and $B_{j,k+1} = (T - \lambda_j I) B_{jk}$. $\square$

The general formula (9.1) implies that the coefficients $\alpha_0^{(k)}, \alpha_1^{(k)}$ which solve (4.1), (4.1′) are the solution of the linear system

(11.2) $$\begin{pmatrix} (\eta_k, \eta_k), & (\eta_{k-n}, \eta_k) \\ (\eta_k, \eta_{k-n}), & (\eta_{k-n}, \eta_{k-n}) \end{pmatrix} \begin{pmatrix} \alpha_0^{(k)} \\ \alpha_1^{(k)} \end{pmatrix} = \nu \begin{pmatrix} 1 \\ 1 \end{pmatrix},$$

(11.2′) $$\alpha_0^{(k)} + \alpha_1^{(k)} = 1\,.$$

It was proved in [1] that there exists an integer $k_1 \geqq k_0$ such that for every $k > k_1$ the matrix of the system (11.2) is positive definite, and if the dimension of X is finite, then we can put $k_1 = k_0$. In [1] (see Theorem 3 and Lemma 4) this assertion is proved for every integer $l < \sum_{j=1}^{r} i_j$.

If we use the notation $\delta_1 \eta_k$ for the difference

(12.2) $$\delta_1 \eta_k = \eta_k - \eta_{k-n}$$

then (11.2) and (11.2′) yield

(13.2) $$\begin{aligned}(\delta_1\eta_k, \delta_1\eta_k)\,\alpha_0^{(k)} &= -(\eta_{k-n}, \delta_1\eta_k)\,,\\ (\delta_1\eta_k, \delta_1\eta_k)\,\alpha_1^{(k)} &= (\eta_k, \delta_1\eta_k)\,.\end{aligned}$$

Now we shall describe the asymptotic behaviour of the numbers $(\eta_{k-n}, \delta_1\eta_k)$ and $(\delta_1\eta_k, \delta_1\eta_k)$. The following lemmas will be of assistance in completing the calculations.

Lemma 2.2. *Let $j \in \langle 1, r\rangle$ and μ be integers. If we put $w(k) = k^\mu \lambda_j^{-k}\, v(k)$, where $v(k)$ is defined by* (10.2), *then*

(14.2) $$\lim_{k\to\infty} w(k) = 0\,.$$

Proof. The following inequality is evident:

$$\|k^\mu \lambda_j^{-k}\, v(k)\| \leqq k^\mu |\lambda_j|^{-k}\, \|I - T^n\|\, \frac{1}{2\pi}\, 2\pi\varrho_0\varrho_0^k\,.\max_{|\lambda|=\varrho_0} \|R(\lambda, T)\|\, \|\varepsilon_0\| =$$

$$= (\|I - T^n\|\, \varrho_0 \max_{|\lambda|=\varrho_0} \|R(\lambda, T)\|\, \|\varepsilon_0\|)\, k^\mu \left(\frac{\varrho_0}{|\lambda_j|}\right)^k .$$

The relation (14.2) now follows from the fact that $\varrho_0 < |\lambda_j|$. □

Remark. Let $\nu \geqq 0$ be an arbitrary integer, $\mathbf{u} = \{u_k\}_{k=\nu}^\infty$, $\mathbf{v} = \{v_k\}_{k=\nu}^\infty$ two sequences. The symbol $\mathbf{u} = O(v_k)$ denotes that $|u_k| \leqq c|v_k|$ for some constant c for all $k \geqq \nu$. If $\mathbf{u} = O(v_k)$ and $\mathbf{v} = O(u_k)$ then we will write $\mathbf{u} \cong \mathbf{v}$.

Lemma 3.2. *If k and i, where $k > n$ and $1 \leqq i \leqq k - n + 1$, are positive integers then the equality*

(15.2) $$\binom{k}{i-1}^{-1}\binom{k-n}{i-1} = 1 - \frac{n(i-1)}{k} + \varphi_k \quad \textit{holds}\,,$$

where $\varphi = \{\varphi_k\}_{k=n-1+i}^\infty = O(1/k^2)$. Moreover, $\varphi \equiv 0$ if $i = 1$.

Proof. The assertion is evident for $i = 1$. For $i > 1$ we have

$$\binom{k}{i-1}^{-1}\binom{k-n}{i-1} = \left(1 - \frac{n}{k}\right)\left(1 - \frac{n}{k-1}\right)\dots\left(1 - \frac{n}{k-i+2}\right) =$$

$$\left(1 - \frac{n}{k}\right)\left(1 - \frac{n}{k}\sum_{s=0}^\infty\left(\frac{1}{k}\right)^s\right)\dots\left(1 - \frac{n}{k}\sum_{s=0}^\infty\left(\frac{i-2}{k}\right)^s\right) = 1 - \frac{n}{k}(i-1) + \varphi_k\,,$$

where evidently $\{\varphi_k\}_{k=n+i}^{\infty} = O(1/k^2)$. □

For the vector η_k defined by (5.1) we have obtained the expression (9.2). Analogously we can obtain a formula for η_{k-n}.

Lemma 4.2. *Assuming as before that $k \geqq k_0$ then the vector η_{k-n} satisfies the formula*

$$\eta_{k-n} = \lambda_1^{k-n} v_{11} + \sum_{j=2}^{r} \sum_{i=1}^{i_j} \binom{k}{i-1} \lambda_j^{k-n} a_{ji}(k) + v(k-n)\,, \tag{16.2}$$

where

$$a_{ji}(k) = \left(1 - \frac{n(i-1)}{k} + \varphi_{ji}(k)\right) v_{ji} \quad \text{and} \quad \{\varphi_{ji}(k)\}_{k=k_0}^{\infty} = O\left(\frac{1}{k^2}\right) \tag{17.2}$$

for all j, i. Moreover, $\{\varphi_{ji}(k)\}_{k=k_0}^{\infty} \equiv 0$ for $i = 1$.

Proof. In (9.2) we replace k by $k - n$ and apply Lemma 3.2. □

Denoting

$$\sum_{i=1}^{i_j}{}' \cdot = \begin{cases} \sum_{i=1}^{i_j-1} \cdot & \text{if } j = 2 \\ \sum_{i=1}^{i_j} \cdot & \text{if } j > 2\,, \end{cases}$$

we obtain from (12.2), (9.2) and (16.2) that

$$\delta_1 \eta_k = \eta_k - \eta_{k-n} = \tag{18.2}$$

$$= \lambda_1^k v_{11} + \binom{k}{i_2 - 1} \lambda_2^k \left[v_{2i_2} + \binom{k}{i_2-1}^{-1} \lambda_2^{-k} \left\{ \sum_{j=2}^{r} \sum_{i=1}^{i_j}{}' \binom{k}{i-1} \lambda_j^k v_{ji} + v(k) \right\} \right] -$$

$$- \lambda_1^{k-n} v_{11} - \binom{k}{i_2 - 1} \lambda_2^{k-n} \left[a_{2i_2}(k) + \right.$$

$$\left. + \binom{k}{i_2-1}^{-1} \lambda_2^{-k+n} \left\{ \sum_{j=2}^{r} \sum_{i=1}^{i_j}{}' \binom{k}{i-1} \lambda_j^{k-n} a_{ji}(k) + v(k-n) \right\} \right].$$

In order to simplify the formula (18.2) we introduce

Assumption 2. *Either*

(A1) $\quad (v_{11}, v_{2i_2}) \neq 0$ *or*

(A2) $\quad (v_{11}, v_{ji}) = 0$ *for all* $j > 1$, $1 \leqq i \leqq i_j$. □

This assumption makes the formulas for η_{k-n} and $\delta_1 \eta_k$ much simpler.

Lemma 5.2. *There exist sequences of vectors $\{u_1(k)\}_{k=k_0-n}^{\infty} \subset X$ and $\{u_2(k)\}_{k=k_0}^{\infty} \subset X$ such that for $k \geqq k_0$ the relations*

$$\eta_{k-n} = \lambda_1^{k-n} v_{11} + \binom{k}{i_2-1} \lambda_2^{k-n} [v_{2i_2} + u_1(k-n)]\,, \tag{19.2}$$

(20.2) $$\delta_1\eta_k = \lambda_1^k(1-\lambda_1^{-n})\,v_{11} + \binom{k}{i_2-1}\lambda_2^k(1-\lambda_2^{-n})\,[v_{2i_2} + u_2(k)]\,,$$

(21.2) $$\{\|u_s(k)\|\}_{s=k_0}^{\infty} = O\left(\frac{1}{k}\right) \quad \text{if} \quad i_2 > 1\,,$$

(22.2) $$\{\|u_s(k)\|\}_{s=k_0}^{\infty} = O\left(k^{i_3-1}\left(\frac{\lambda_3}{\lambda_2}\right)^k\right) \quad \text{if} \quad i_2 = 1$$

hold. The relations (21.2) *and* (22.2) *are valid for* $s = 1, 2$.

Proof. The statements (19.2) and (20.2) follow immediately from (16.2), (17.2), (18.2).

3. EXPLICIT FORMULAS FOR COEFFICIENTS $\alpha_0^{(k)}$ AND $\alpha_1^{(k)}$

From (19.2) and (20.2) we easily obtain formulas for the scalar products $(\eta_{k-n}, \delta_1\eta_k)$ and $(\delta_1\eta_k, \delta_1\eta_k)$. The structure of the spectrum of the operator T was described in the previous part. We suppose the assumptions 1 and 2 are valid. For the sake of simplicity we put

(1.3) $$\frac{\lambda_2}{\lambda_1} = q\,e^{i\varphi}\,, \quad \text{where} \quad q = \left|\frac{\lambda_2}{\lambda_1}\right|.$$

The integer k_0 was defined by (7.2).

Lemma 1.3. *There exist sequences of complex numbers* $\{\beta_k\}_{k=k_0}^{\infty} = O(1)$ *and* $\{\gamma_k\}_{k=k_0}^{\infty} = O(1)$ *and positive integers* $\varkappa_1, \varkappa_2$ *such that the equalities*

(2.3) $$(\eta_{k-n}, \delta_1\eta_k) = \lambda_1^{2k}\,\lambda_1^{-n}(1-\lambda_1^{-n})\,\|v_{11}\|^2\,[1 + k^{\varkappa_1}q^{\varkappa_2 k}\beta_k]\,,$$

(3.3) $$(\delta_1\eta_k, \delta_1\eta_k) = \lambda_1^{2k}\,|1-\lambda_1^{-n}|^2\,\|v_{11}\|^2\,[1 + k^{\varkappa_1}q^{\varkappa_2 k}\gamma_k]$$

hold. If the case (A1) *holds in assumption* 2 *then* $\varkappa_1 = i_2 - 1$ *and* $\varkappa_2 = 1$. *If, moreover,* λ_2 *is real then*

(4.3) $$\{\beta_k\}_{k=k_0}^{\infty} \cong \{1\}\,,$$

and if $(v_{11}, v_{2i_2}) \neq \mathrm{i}d$ *for some real* d *then*

(4.3') $$\{\gamma_k\}_{k=k_0}^{\infty} \cong \{1\}\,.$$

If (A2) *holds then* $\varkappa_1 = 2(i_2-1)$, $\varkappa_2 = 2$ *and the relations* (4.3) *and* (4.3') *hold.*

Proof. First, we shall prove (2.3). From (19.2) and (20.2) it is obvious that

$$(\eta_{k-n}, \delta_1\eta_k) = |\lambda_1|^{2k}\,\lambda_1^{-n}(1-\lambda_1^{-n})\,(v_{11}, v_{11}) +$$
$$+ \lambda_1^{k-n}\bar{\lambda}_2^k\binom{k}{i_2-1}\overline{(1-\lambda_2^{-n})}\,(v_{11}, v_{2i_2} + u_2(k)) +$$

$$+ \lambda_1^k \lambda_2^{k-n} \binom{k}{i_2 - 1} (1 - \lambda_1^{-n}) (v_{2i_2} + u_1(k - n), v_{11}) +$$

$$+ \binom{k}{i_2 - 1}^2 \lambda_2^{-n} |\lambda_2|^{2k} \overline{(1 - \lambda_2^{-n})} (v_{2i_2} + u_1(k - n), v_{2i_2} + u_2(k)) .$$

Since we have $\binom{k}{i_2 - 1} = \frac{1}{(i_2 - 1)!} k^{i_2 - 1} \left(1 - \frac{1}{k}\right) \left(1 - \frac{2}{k}\right) \dots \left(1 - \frac{i_2 - 2}{k}\right) =$

$= k^{i_2 - 1} \left(\frac{1}{(i_2 - 1)!} + \psi_k \right)$, for $i_2 \geqq 1$ and $k > k_0$, where $\{\psi_k\}_{k=k_0}^{\infty} = O\left(\frac{1}{k}\right)$ if $i_2 > 1$ and $\{\psi_k\} \equiv 0$ for $i_2 = 1$, we obtain by easy calculation

$$(\eta_{k-n}, \delta_1 \eta_k) = \lambda_1^{2k} \lambda_1^{-n} \overline{(1 - \lambda_1^{-n})} \|v_{11}\|^2 \Big[1 + k^{i_2 - 1} q^k \{ e^{-ik\varphi} \frac{\overline{1 - \lambda_2^{-n}}}{1 - \lambda_1^{-n}} (v_{11}, v_{2i_2}) +$$

$$(5.3) \qquad + e^{ik\varphi} \frac{\lambda_2^{-n}}{\lambda_1^{-n}} (v_{2i_2}, v_{11}) + \vartheta_1(k) \} / \|v_{11}\|^2 / (i_2 - 1)! +$$

$$+ k^{2(i_2 - 1)} q^{2k} \left\{ \frac{\lambda_2^{-n}}{\lambda_1^{-n}} \frac{\overline{1 - \lambda_2^{-n}}}{1 - \lambda_1^{-n}} (v_{2i_2}, v_{2i_2}) + \vartheta_2(k) \right\} \Big/ \|v_{11}\|^2 / ((i_2 - 1)!)^2 \Big] ,$$

where according to Lemma 5.2

$$\{\vartheta_s(k)\}_{k=k_0}^{\infty} = \begin{cases} O\left(\frac{1}{k}\right) & \text{if} \quad i_2 > 1 \\ O\left(k^{i_3 - 1} \left(\frac{\lambda_3}{\lambda_2}\right)^k\right) & \text{if} \quad i_2 = 1 \end{cases}$$

for $s = 1. 2$. Putting

(6.3)

$$\beta_k^{(1)} = \left\{ e^{-ik\varphi} \frac{\overline{1 - \lambda_2^{-n}}}{1 - \lambda_1^{-n}} (v_{11}, v_{2i_2}) + e^{ik\varphi} \frac{\lambda_2^{-n}}{\lambda_1^{-n}} (v_{2i_2}, v_{11}) + \vartheta_1(k) \right\} \Big/ \|v_{11}\|^2 / (i_2 - 1)! ,$$

$$(7.3) \qquad \beta_k^{(2)} = \left\{ \frac{\lambda_2^{-n}}{\lambda_1^{-n}} \frac{\overline{1 - \lambda_2^{-n}}}{1 - \lambda_1^{-n}} (v_{2i_2}, v_{2i_2}) + \vartheta_2(k) \right\} \Big/ \|v_{11}\|^2 / ((i_2 - 1)!)^2 ,$$

we have from (5.3)

$$(8.3) \qquad (\eta_{k-n}, \delta_1 \eta_k) = \lambda_1^{2k} \lambda_1^{-n} (1 - \lambda_1^{-n}) \|v_{11}\|^2 [1 + k^{i_2 - 1} q^k (\beta_k^{(1)} + k^{i_2 - 1} q^k \beta_k^{(2)})] .$$

Substituting in this formula

$$(9.3) \qquad \beta_k = \beta_k^{(1)} + k^{i_2 - 1} q^k \beta_k^{(2)}$$

we immediately obtain (2.3). The relation $\{\beta_k\}_{k=k_0}^{\infty} = O(1)$ follows evidently from (6.3), (7.3) and (9.3). Assuming (A1) and λ_2 real we have

$$|\beta_k^{(1)}| \geqq \left| \left| \frac{1 - \lambda_2^{-n}}{1 - \lambda_1^{-n}} \right| - \left| \frac{\lambda_2^{-n}}{\lambda_1^{-n}} \right| \right| \frac{|(v_{11}, v_{2i_2})|}{\|v_{11}\|^2} - |\vartheta_1(k)| .$$

But $\vartheta_1(k) \to 0$ and $k^{i_2-1}q^k\beta_k^{(2)} \to 0$ and therefore in order to prove (4.3) it is sufficient to show that $|(1-\lambda_2^{-n})/(1-\lambda_1^{-n})| - |\lambda_2^{-n}/\lambda_1^{-n}| \neq 0$. Evidently we have

$$\frac{1-\lambda_2^{-n}}{1-\lambda_1^{-n}} - \frac{\lambda_2^{-n}}{\lambda_1^{-n}} \neq 0 \quad \text{and} \quad \frac{1-\lambda_2^{-n}}{1-\lambda_1^{-n}} + \frac{\lambda_2^{-n}}{\lambda_1^{-n}} \neq 0\,.$$

If assumption (A2) is fulfilled then $\beta_k^{(1)} = 0$, and substituting $\beta_k = \beta_k^{(2)}$ in (8.3) we obtain (2.3). From (7.3) we have

$$\liminf_{k\to\infty} |\beta_k| = \left|\frac{\lambda_2^{-n}}{\lambda_1^{-n}}\right| \left|\frac{1-\lambda_2^{-n}}{1-\lambda_1^{-n}}\right| \frac{\|v_{2i_2}\|^2}{\|v_{11}\|^2\,((i_2-1)!)^2} > 0\,.$$

Analogously we can construct numbers

$$\gamma_k^{(1)} = \left\{ e^{-ik\varphi}\,\overline{\frac{1-\lambda_2^{-n}}{1-\lambda_1^{-n}}}\,(v_{11}, v_{2i_2}) + e^{ik\varphi}\,\frac{1-\lambda_2^{-n}}{1-\lambda_1^{-n}}\,(v_{2i_2}, v_{11}) + \vartheta_1'(k)\right\} \Big/ \|v_{11}\|^2/(i_2-1)!\,, \tag{10.3}$$

$$\gamma_k^{(2)} = \left(\left|\frac{1-\lambda_2^{-n}}{1-\lambda_1^{-n}}\right|^2 \|v_{2i_2}\|^2 + \vartheta_2'(k)\right) \Big/ \|v_{11}\|^2/((i_2-1)!)^2\,, \tag{11.3}$$

where $\{\vartheta_s'(k)\}_{k=k_0}^{\infty}$ equals $O(1/k)$ or $O(k^{i_3-1}(\lambda_3/\lambda_2)^k)$ in the same way as $\{\vartheta_s(k)\}_{k=k_0}^{\infty}$. Putting

$$\gamma_k = \gamma_k^{(1)} + k^{i_2-1}\gamma_k^{(2)} \tag{12.3}$$

we have (3.3). The rest of the proof is obvious. □

The relations (6.3)–(12.3) imply that

$$\hat{\delta}_k = \beta_k - \gamma_k = e^{ik\varphi}\left(\frac{\lambda_2^{-n}}{\lambda_1^{-n}} - \frac{1-\lambda_2^{-n}}{1-\lambda_1^{-n}}\right)(v_{2i_2}, v_{11})/\|v_{11}\|^2/(i_2-1)! + \vartheta_3(k) + k^{i_2-1}q^k \left\{\overline{\frac{1-\lambda_2^{-n}}{1-\lambda_1^{-n}}}\left(\frac{\lambda_2^{-n}}{\lambda_1^{-n}} - \frac{1-\lambda_2^{-n}}{1-\lambda_1^{-n}}\right)\frac{\|v_{2i_2}\|^2}{\|v_{11}\|^2\,((i_2-1)!)^2} + \vartheta_3'(k)\right., \tag{13.3}$$

where $\{\vartheta_3(k)\}$, $\{\vartheta_3'(k)\}$ equals $O(1/k)$ or $O((\lambda_3/\lambda_2)^k k^{i_3-1})$. Evidently

$$\limsup_{k\to\infty} |\hat{\delta}_k| < +\infty \quad \text{and for a real } \lambda_2 \text{ we have} \tag{14.3}$$

$$\liminf_{k\to\infty} |\hat{\delta}_k| > 0\,. \tag{14.3'}$$

From (13.2) and Lemma 1.3 it follows that

$$\alpha_0^{(k)} = -\frac{(\eta_{k-n}, \delta_1\eta_k)}{(\delta_1\eta_k, \delta_1\eta_k)} = \frac{1}{1-\lambda_1^n}\,(1 + k^{\varkappa_1}q^{\varkappa_2 k}\delta_k)\,, \tag{15.3}$$

where

$$\delta_k = \hat{\delta}_k + \vartheta_4(k) \quad \text{and} \quad \{\vartheta_4(k)\} = O(k^{\varkappa_1}q^{\varkappa_2 k})\,. \tag{16.3}$$

From (11.2′) it follows that

$$\alpha_1^{(k)} = -\frac{\lambda_1^n}{1-\lambda_1^n}\left(1 + k^{\varkappa_1} q^{\varkappa_2 k} \vartheta_k\right), \tag{17.3}$$

where

$$\vartheta_k = \delta_k / \lambda_1^n \,. \tag{17.3′}$$

This all is valid not only for sufficiently great k but for all $k \geqq k_0$ as we shall see in Part 4.

Remark. Assumption 2 is no restriction. Supposing some other orthogonal relations to hold between v_{ji}, we obtain for $\alpha_0^{(k)}$ and $\alpha_1^{(k)}$ the formulas (15.3) and (17.3) again where $\varkappa_1$ is a nonnegative integer (in general $\varkappa_1 \neq i_2 - 1$) and $|q| < 1$ (in general $|q| \neq |\lambda_2/\lambda_1|$). The other relations are valid.

Let us summarize all the results.

Theorem 1.3. *Let X be a Hilbert space, $T \in [X]$, $r(T) < 1$. Let $\lambda_1, \ldots, \lambda_r$ be poles of $R(\lambda, T)$ of order $i_1, \ldots, i_r$, respectively, and suppose that (1.2)–(7.2) and Assumption 2 are valid. Let us denote $q = |\lambda_2/\lambda_1|$.*

Then there exist sequences $\{\delta_k\}_{k=k_0}^{\infty} = O(1)$ and $\{\vartheta_k\}_{k=k_0}^{\infty} = O(1)$ such that

$$\alpha_0^{(k)} = \frac{1}{1-\lambda_1^n}\left(1 + k^{\varkappa_1} q^{\varkappa_2 k} \delta_k\right),$$

$$\alpha_1^{(k)} = -\frac{\lambda_1^n}{1-\lambda_1^n}\left(1 + k^{\varkappa_1} q^{\varkappa_2 k} \vartheta_k\right), \quad \text{where} \quad \vartheta_k = \delta_k/\lambda_1^n \,.$$

If (A1) in Assumption 2 is valid, then $\varkappa_1 = i_2 - 1$ and $\varkappa_2 = 1$. If (A2) in Assumption 2 is valid, then $\varkappa_1 = 2(i_2 - 1)$ and $\varkappa_2 = 2$. If, moreover, λ_2 is real then $\{\delta_k\}_{k=k_0}^{\infty} \cong \{1\}$ in both cases.

4. CALCULATION OF λ_1 AND λ_2

The question to be considered in this section is that of finding the poles λ_1 and λ_2. The equations (15.3) and (17.3) provide formulas not only for the calculation of λ_1 but, also as we shall see, for λ_2. However (15.3) and (17.3) imply only that $\alpha_0^{(k)} \neq 0$ for all $k \geqq k_1$, where k_1 is an integer greater than k_0 defined by (7.2). According to (13.2), as a first step toward the expression of λ_1 and λ_2, it will be shown that in general $\eta_k \neq 0$ and $\delta_1 \eta_k \neq 0$ for all $k \geqq k_0$. Let us assume the contrary.

Lemma 1.4. *If for some $k_1 \geqq k_0$ the relation $\eta_{k_1 - n} = 0$ holds then $x_{k_1} = x^* = Tx^* + b$.* □

The proof is obvious.

It is natural to introduce

Assumption 3. *Let the iterative process (2.1) be not finished after a finite number of steps, i.e. let the equality $x_{k_1} = x^*$ be not valid for any $k_1 \geqq k_0$.*

Lemma 2.4. *Let Assumption* 3 *be valid. Then*

$$\eta_k \neq 0 \quad \text{and} \quad \delta_1 \eta_k \neq 0 \tag{1.4}$$

for all $k \geqq k_0 = \max_{j=1,\ldots,r} (i_j) + n$. □

The proof is obvious.

Asumption 3 makes it possible to define a sequence $\{\lambda_1(n, k)\}_{k=k_0}^{\infty}$ by the formula

$$\lambda_1(n, k) = -\alpha_1^{(k)}/\alpha_0^{(k)} . \tag{2.4}$$

Theorem 1.3 implies

$$\lambda_1(n, k) = \lambda_1^n \left[1 + k^{\varkappa_1} q^{\varkappa_2 k} \frac{\vartheta_k - \delta_k}{1 + k^{\varkappa_1} q^{\varkappa_2 k} \delta_k} \right]. \tag{3.4}$$

If we denote

$$\xi_k = (1 - \lambda_1^n) \frac{\delta_k}{1 + k^{\varkappa_1} q^{\varkappa_2 k} \delta_k} \tag{4.4}$$

then using (3.4), (13.3) and (17.3′) we can formulate the following theorem.

Theorem 1.4. *Let us suppose that the assumptions of Theorem* 1.3 *and Assumption* 3 *are satisfied. Let* $\{\lambda_1(n, k)\}_{k=k_0}^{\infty}$ *be defined by* (2.4). *Then there exists a sequence* $\{\xi_k\}_{k=k_0}^{\infty} = O(1)$ such that

$$\lambda_1(n, k) = \lambda_1^n + k^{\varkappa_1} q^{\varkappa_2 k} \xi_k \tag{5.4}$$

holds. The numbers $\varkappa_1$, $\varkappa_2$ *and* q *are the same as above in Theorem* 1.3.

Let, moreover, λ_2 *be real. If* (A1) *is valid and if we denote*

$$\delta = \left(\frac{\lambda_2^{-n}}{\lambda_1^{-n}} - \frac{1 - \lambda_2^{-n}}{1 - \lambda_1^{-n}} \right) \frac{(v_{2i_2}, v_{11})}{\|v_{11}\|^2 (i_2 - 1)!}, \tag{6.4}$$

then

$$\xi_k = (1 - \lambda_1^{-n}) \delta + \vartheta_{4,1}(k) . \tag{7.4}$$

If (A2) *is valid and if we denote*

$$\delta' = \frac{1 - \lambda_2^{-n}}{1 - \lambda_1^{-n}} \left(\frac{\lambda_2^{-n}}{\lambda_1^{-n}} - \frac{1 - \lambda_2^{-n}}{1 - \lambda_1^{-n}} \right) \frac{\|v_{2i_2}\|^2}{\|v_{11}\|^2 ((i_2 - 1)!)^2} \tag{6.4′}$$

then

$$\xi_k = (1 - \lambda_1^n) \delta' + \vartheta_{4,2}(k) . \tag{7.4′}$$

In both cases, for $s = 1, 2$ *we have*

$$\vartheta_{4,s}(k) = \begin{cases} O\left(\frac{1}{k}\right) & \text{if} \quad i_2 > 1 \\ O\left(\max\left[\left(\frac{\lambda_2}{\lambda_1}\right)^k, k^{i_3 - 1}\left(\frac{\lambda_3}{\lambda_2}\right)^k\right]\right) & \text{if} \quad i_2 = 1 \end{cases}$$

and $\{\xi_k\}_{k=k_0}^{\infty} \cong \{1\}$. □

From (19.2) we have

$$\omega_k^{(1)} \stackrel{\text{def}}{=} \eta_k - \lambda_1^n \eta_{k-n} = k^{i_2-1}\lambda_2^k \left(1 - \frac{\lambda_2^{-n}}{\lambda_1^{-n}}\right)(v_{2i_2}/(i_2-1)! + u_k) \tag{8.4}$$

where

$$\{\|u_k\|\}_{k=k_0}^{\infty} = \begin{cases} O\left(\frac{1}{k}\right) & \text{if } i_2 > 1 \\ O\left(\left(\frac{\lambda_3}{\lambda_2}\right)^k k^{i_3-1}\right) & \text{if } i_2 = 1 . \end{cases}$$

However, what happens if we do not know λ_1 a priori? We should use only $\lambda_1(k, n)$ instead of λ_1 in this case. Substituting (5.4) in (8.4) gives

$$\omega_k \stackrel{\text{def}}{=} \eta_k - \lambda_1(n, k)\, \eta_{k-n} = \tag{9.4}$$

$$= \omega_k^{(1)} - k^{\varkappa_1} q^{\varkappa_2 k} \xi_k [\lambda_1^{k-n} v_{11} + k^{i_2-1} \lambda_2^{k-n}(v_{2i_2}/(i_2-1)! + u_1(k-n)] ,$$

where $\{\|u_1(k-n)\|_{k=k_0}^{\infty}$ equals $O\left(\frac{1}{k}\right)$ or $O\left(\left(\frac{\lambda_3}{\lambda_2}\right)^k k^{i_3-1}\right)$.

We are interested in the second term on the right hand side of (9.4). We have $q = |\lambda_2/\lambda_1|$ and if Assumption 2 is not valid, the inequality $q < |\lambda_2/\lambda_1|$ may hold. This inequality implies that $\omega_k = \omega_k^{(1)} + o((\lambda_2/\lambda_1)^k)$ for $k \to \infty$ and the same is true if $\varkappa_2 = 2$. Hence (A1) in Assumption 2 represents the most pessimistic case. In the sequel, let (A1) hold. We have

$$\omega_k = \omega_k^{(1)} - k^{i_2-1} \left\{\left(\frac{\lambda_2}{\lambda_1}\right)^k e^{-ik\varphi} \xi_k \lambda_1^{k-n} v_{11} + \lambda_2^k \tilde{u}_k\right\},$$

where $\{\|\tilde{u}_k\|\} = O(k^{i_2-1}(\lambda_2/\lambda_1)^k)$.

Substituting $\omega_k^{(1)}$ from (8.4) we obtain

$$\omega_k = k^{i_2-1}\lambda_2^k \left[\frac{\lambda_1^{-n} - \lambda_2^{-n}}{\lambda_1^{-n}(i_2-1)!} v_{2i_2} - e^{-ik\varphi}\, \xi_k \lambda_1^{-n} v_{11} + z_k\right], \tag{10.4}$$

where the sequence $\{\|z_k\|\}_{k=k_0}^{\infty}$ behaves in the same way as $\{\vartheta_{4,1}(k)\}$ in (7.4). If λ_2 is real, then we can put $(1 - \lambda_1^{-n})\,\delta$ instead of ξ_k. The above considerations yield.

Theorem 2.4. *Let us suppose that the assumptions of Theorem* 1.4 *are satisfied. Then there exist sequences* $\{w_k\}_{k=k_0}^{\infty}$ *and* $\{z_k\}_{k=k_0}^{\infty}$ *such that*

$$\{\|w_k\|\}_{k=k_0}^{\infty} = O(1) , \quad w_k \neq 0 \quad \forall k \geqq k_0 , \tag{11.4}$$

$$\{\|z_k\|\}_{k=k_0}^{\infty} = \begin{cases} O\left(\frac{1}{k}\right) & \textit{if } i_2 > 1 \\ O\left(\max\left[\left(\frac{\lambda_2}{\lambda_1}\right)^k, \; k^{i_3-1}\left(\frac{\lambda_3}{\lambda_2}\right)^k\right]\right) & \textit{if } i_2 = 1 , \end{cases} \tag{12.4}$$

and the equality

$$\omega_k = k^{i_2-1}\lambda_2^k(w(k) + z(k)) \tag{13.4}$$

holds. If λ_2 is real then $w(k) \equiv w \neq 0$ is independent of k. Moreover,

$$\frac{(\omega_{k+n}, \omega_{k+n})}{(\omega_k, \omega_k)} = |\lambda_2|^{2n} + v(k) \tag{14.4}$$

and

$$\frac{(\omega_{k+n}, \omega_k)}{(\omega_k, \omega_k)} = \lambda_2^n + v_1(k)\,, \tag{15.4}$$

where the behaviour of the sequences $\{v(k)\}$ and $\{v_1(k)\}$ is the same as above in (12.4). □

5. BEHAVIOUR OF AN EXTRAPOLATED VECTOR

Concluding our theoretical investigation we give an explicit formula for the vector $y_k = \alpha_0^{(k)}x_k + \alpha_1^{(k)}x_{k-n}$. Denoting

$$u_{ji} = B_{ji}\varepsilon_0/\lambda_j^{i-1} \tag{1.5}$$

we obtain from (8.2), (19.2) and (5.1) that

$$x_k = x^* - \{\lambda_1^k u_{11} + k^{i_2-1}\lambda_2^k[u_{2i_2} + z_1(k)]\} \tag{2.5}$$

where $\{\|z_1(k)\|\}$ equals $O(1/k)$ or $O\left(\left(\frac{\lambda_3}{\lambda_2}\right)^k k^{i_3-1}\right)$

depending on i_2 as above.
Hence, using (15.3) and (17.3), we have

$$\begin{aligned} y_k &= \alpha_0^{(k)}x_k + \alpha_1^{(k)}x_{k-n} = \\ &= x^* + k^{i_2-1}\lambda_2^k\left[\left\{(\lambda_1^{-n} - 1)\,\delta_k u_{11} + \left(\frac{\lambda_2^{-n}}{\lambda_1^{-n}} - 1\right)u_{2i_2}\right\}\Big/(1 - \lambda_1^n) + z_k\right], \end{aligned} \tag{3.5}$$

where the behaviour of $\{\|z_k\|\}$ is given by (12.4).

Theorem 1.5. *Let us suppose that the assumptions of Theorem* 1.4 *are satisfied. Then there exist sequences $\{w_k\}_{k=k_0}^{\infty}$ and $\{z_k\}_{k=k_0}^{\infty}$ with the same behaviour as in Theorem* 2.4, *such that*

$$y_k - x^* = k^{i_2-1}\lambda_2^k(w_k + z_k) \tag{4.5}$$

holds. If λ_2 is real then $w_k \equiv w \neq 0$ is independent of k.

Moreover, there exists a sequence $\{z_{1k}\}_{k=k_0}^{\infty}$ such that $\{\|z_{1k}\|\} = O(k^{i_2-1}(\lambda_2/\lambda_1)^k)$,

$$y_{k+1} - x^* = T(y_k - x^*) + z_{1k} \tag{5.5}$$

and

$$y_{k+1} = Ty_k + b + z_{1k}\,. \qquad (6.5) \qquad \square$$

Proof. The statement of this theorem follows from (15.3), (17.3) and the calculations at the beginning of this section.

6. OPTIMAL CONVERGENCE OF EXTRAPOLATED S.O.R.

In this section we show how the above results can be applied for improving the convergence of the optimal S.O.R. without any a priori knowledge of eigenvalues of the corresponding Jacobi and S.O.R. matrices, respectively. Let X be the t-dimensional space. We seek the solution of the matrix equation

$$Ax = b\,, \qquad (1.6)$$

where A is a given $t \times t$ positive definite matrix, $t \geqq 4$. Let us write

$$A = D(I - L - U)\,, \qquad (2.6)$$

where D is the diagonal of A, while L and U are strictly lower and upper triangular matrices, respectively. The system (1.6) is equivalent to the system

$$x = \mathscr{L}_\omega x + d\,, \qquad (3.6)$$

where

$$\mathscr{L}_\omega = (I - \omega L)^{-1}(\omega U + (1 - \omega) D) \quad \text{and} \quad d = \omega(I - \omega L)^{-1} D^{-1} b\,. \qquad (4.6)$$

It is well known that $r(\mathscr{L}_\omega) < 1$ for $\omega \in (0, 2)$. We assume that the Jacobi matrix B is weakly cyclic of index 2, consistently ordered and convergent. If

$$\mu_1 > \mu_2 > \ldots > \mu_p \qquad (5.6)$$

are all mutually different positive eigenvalues of B then the spectrum $\sigma(B)$ satisfies (see [6], [7], [4])

$$\sigma(B) \dot{-} \{0\} = \{\mu_1, \ldots, \mu_p, -\mu_1, \ldots, -\mu_p\}\,. \qquad (6.6)$$

Put $\mu_i^2 = \nu_i$. It is well known (see [6]) that

$$\sigma(\mathscr{L}_1) \dot{-} \{0\} = \{\nu_1, \ldots, \nu_p\}\,. \qquad (7.6)$$

Let f be a mapping, $\mathscr{D}(f) = (0, 1)$, given by the formula

$$f(x) = 2/(1 + \sqrt{(1 - x)})\,. \qquad (8.6)$$

Evidently $\mathbb{R}(f) = (1, 2)$. The numbers $\omega_i = f(\nu_i)$ will be called i-optimal and the numbers from the set $(1, 2) \dot{-} \{\omega_i | i = 1, \ldots, p\}$ will be called regular. The function $r(\mathscr{L}_\omega)$ is continuous in the interval $(0, 2)$, decreases in $(0, \omega_1\rangle$ and coincides with the function $\omega - 1$ in $\langle\omega_1, 2)$ and $r(\mathscr{L}_2) = 1$. Hence

$$\min\{r(\mathscr{L}_\omega) \mid \omega \in (0, 2)\} = \omega_1 - 1 < 1 \qquad (10.6)$$

From (8.6) it follows that

$$1 < \omega_p < \omega_{p-1} < \ldots < \omega_1 < 2 . \tag{11.6}$$

For any ω_j we have $\omega_j^2 \mu_j^2 - 4(\omega - 1) = 0$. The following theorem has been proved in [6]. We only present it in a form suitable for our purposes.

Theorem 1.6. *If $\omega \in (1, 2)$ is regular, then $\mathscr{L}_\omega$ is normalizable and the number*

$$\lambda_{2j-1}(\omega) = ((\omega\mu_j + \sqrt{(\omega^2\mu_j^2 - 4(\omega - 1))})/2)^2 , \tag{13.6}$$

$$\lambda_{2j}(\omega) = ((\omega\mu_j - \sqrt{(\omega^2\mu_j^2 - 4(\omega - 1))})/2)^2 \tag{14.6}$$

for $j = 1, \ldots, p$ and $\lambda = 1 - \omega$ if $0 \in \sigma(B)$ are eigenvalues of $\mathscr{L}_\omega$ while no other complex number is an eigenvalue of $\mathscr{L}_\omega$. The multiplicity of $\lambda_{2j-1}(\omega)$ and $\lambda_{2j}(\omega)$ equals the multiplicity of μ_j.

If an integer $i \in \langle 1, p \rangle$, then the matrix $\mathscr{L}_{\omega_i}$ is not normalizable. In this case $\mathscr{L}_{\omega_i}$ possesses d_i principal vectors each of grade 2, where d_i is the multiplictty of the eigenvalue μ_i. All the other eigenvalues of $\mathscr{L}_{\omega_i}$ are simple poles of the resolvent matrix $R(\lambda, \mathscr{L}_{\omega_i})$. For an integer $j \in \langle 1, p \rangle$ and $\omega \in (0, \omega_j\rangle$ the eigenvalues $\lambda_1(\omega)$, $\lambda_2(\omega), \ldots, \lambda_{2j-1}(\omega), \lambda_{2j}(\omega)$ of $\mathscr{L}_\omega$ are real and fulfil the inequalities

$$\lambda_1(\omega) > \lambda_3(\omega) > \ldots > \lambda_{2j-1}(\omega) \geqq \lambda_{2j}(\omega) > \ldots > \lambda_2(\omega) .$$

The equality $\lambda_{2j-1}(\omega) = \lambda_{2j}(\omega)$ holds only for $\omega = \omega_j$.

For any integer $j \in \langle 1, p \rangle$ and real $\omega \in (\omega_j, 2)$ the eigenvalues $\lambda_{2j-1}(\omega), \lambda_{2j}(\omega), \ldots$ $\ldots, \lambda_{2p}(\omega)$ are not real and

$$|\lambda_{2j-1}(\omega)| = |\lambda_{2j}(\omega)| = \ldots = |\lambda_{2p}(\omega)| = \omega - 1 .$$

The last equalities hold for $\omega = \omega_j$, too. □

The proof of this theorem is based on the well known relation between the eigenvalues of B and $\mathscr{L}_\omega$ of the form

$$(\lambda + \omega - 1)^2 = \lambda\omega^2\mu^2 . \tag{15.6}$$

Let us remark that the Jacobi matrix B is normalizable and has real eigenvalues since $D^{1/2}BD^{-1/2} = I - D^{-1/2}AD^{-1/2}$ and the matrix on the right hand side is Hermitian. Theorem 1.6 implies that for $1 \leqq \omega < \omega_2$ the relation (1.2) is valid, and the second eigenvalue $\lambda_3(\omega)$ of $\mathscr{L}_\omega$ is real. In order to verify all essential assumptions in Theorems 1.3, 1.4, 2.4 and 1.5 we must discuss Assumption 2. Therefore, we will discuss the eigenvectors and as the case may be, the principal vectors of $\mathscr{L}_\omega$. For every 2-cyclic matrix A there exists a permutation matrix P such that PAP^{T} has the form

$\begin{pmatrix} D_1, & F \\ E, & D_2 \end{pmatrix}$, where the submatrices D_1 and D_2 are square and diagonal. Since A is positive definite we can form the corresponding Jacobi matrix

(16.6) $$B = \begin{pmatrix} 0, & B_2 \\ B_1, & 0 \end{pmatrix},$$

where $B_1 = D_2^{-1}E$ and $B_2 = D_1^{-1}F$. It suffices to discuss the eigenvectors of B of the form (16.6). Let us remark that all eigenvalues of B are real because A is positive definite.

Theorem 2.6. *Let $\mu_1 \geqq \mu_2 \geqq \ldots \geqq \mu_q$ be all positive eigenvalues of the Jacobi matrix B, and let*

(17.6) $$\begin{pmatrix} v_1 \\ w_1 \end{pmatrix}, \begin{pmatrix} v_2 \\ w_2 \end{pmatrix}, \ldots, \begin{pmatrix} v_q \\ w_q \end{pmatrix}$$

be the corresponding eigenvectors partioned according to (16.6). *Let $z_{2q+1}, \ldots$ $\ldots, z_t$ be the eigenvectors of B corresponding to zero and let $(\lambda_{2j-1}(\omega))^{1/2}$* and *$(\lambda_{2j}(\omega)^{1/2}$ be defined by the formulas*

(18.6) $$(\lambda_{2j-1}(\omega))^{1/2} = (\omega\mu_j + \sqrt{(\omega^2\mu_j^2 - 4(\omega - 1))})/2$$

and

(19.6) $$(\lambda_{2j}(\omega))^{1/2} = (\omega\mu_j - \sqrt{(\omega^2\mu_j^2 - 4(\omega - 1))})/2\,.$$

Then

1) *if ω is regular* (i.e. $\omega \neq \omega_j\ \forall_j = 1, \ldots, q$) *then the vectors*

(20.6) $$\begin{pmatrix} v_1 \\ (\lambda_1(\omega))^{1/2}\, w_1 \end{pmatrix}, \begin{pmatrix} v_2 \\ (\lambda_3(\omega))^{1/2}\, w_2 \end{pmatrix}, \ldots, \begin{pmatrix} v_q \\ (\lambda_{2q-1}(\omega))^{1/2}\, w_q \end{pmatrix},$$
$$\begin{pmatrix} v_1 \\ (\lambda_2(\omega))^{1/2}\, w_1 \end{pmatrix}, \begin{pmatrix} v_2 \\ (\lambda_4(\omega))^{1/2}\, w_2 \end{pmatrix}, \ldots, \begin{pmatrix} v_q \\ (\lambda_{2q}(\omega))^{1/2}\, w_q \end{pmatrix}$$

and $z_{2q+1}, \ldots, z_t$, are the eigenvectors corresponding to the eigenvalues $\lambda_1(\omega), \ldots,$ $\lambda_{2q}(\omega)$ and $1 - \omega$, respectively and form a basis in t-dimensional space;

2) *if ω is* j-*optimal* (i.e. $\omega = \omega_j$ *for some j*) *then $\lambda_{2j-1}(\omega) = \lambda_{2j}(\omega)$. If $\mu_j =$ $= \mu_{j+1} = \ldots = \mu_{j_1}$ and $\mu_j \neq \mu_s\ \forall s \notin \langle j, j_1 \rangle$ then*

(21.6) $$\lambda_{2j-1}(\omega) = \lambda_{2j}(\omega) = \lambda_{2j+1}(\omega) = \ldots = \lambda_{2j_1-1}(\omega) = \lambda_{2j_1}(\omega)\,.$$

The vectors

(22.6) $$\begin{pmatrix} 0 \\ \tfrac{1}{2}(\lambda_{2j}(\omega))^{-1/2}\, w_j \end{pmatrix}, \begin{pmatrix} 0 \\ \tfrac{1}{2}(\lambda_{2j}(\omega))^{-1/2}\, w_{j+1} \end{pmatrix}, \begin{pmatrix} 0 \\ \tfrac{1}{2}(\lambda_{2j}(\omega)^{-1/2}\, w_{j+2} \end{pmatrix}, \ldots$$
$$\ldots, \begin{pmatrix} 0 \\ \tfrac{1}{2}(\lambda_{2j}(\omega))^{-1/2}\, w_{j_1-1} \end{pmatrix}, \begin{pmatrix} 0 \\ \tfrac{1}{2}(\lambda_{2j}(\omega))^{-1/2}\, w_{j_1} \end{pmatrix}$$

are the principal vectors of grade 2 corresponding to the eigenvalue $\lambda_{2j-1}(\omega)$. If we put the vectors (22.6) *in* (20.6) *instead of the vectors*

$$\begin{pmatrix} v_j \\ (\lambda_{2j}(\omega))^{1/2}\, w_j \end{pmatrix}, \begin{pmatrix} v_{j+1} \\ (\lambda_{2j+2}(\omega)^{1/2}\, w_{j+1} \end{pmatrix}, \ldots, \begin{pmatrix} v_{j_1} \\ (\lambda_{2j_1}(\omega))^{1/2}\, w_{j_1} \end{pmatrix}$$

we again obtain a basis in the t-dimensional space. □

This theorem contains results which have been proved in [6], pp. 234–239. If

$$B\begin{pmatrix} v \\ w \end{pmatrix} = \mu\begin{pmatrix} v \\ w \end{pmatrix} \quad \text{for} \quad \begin{pmatrix} v \\ w \end{pmatrix} \neq 0$$

then evidently

$$B\begin{pmatrix} v \\ -w \end{pmatrix} = (-\mu)\begin{pmatrix} v \\ -w \end{pmatrix}.$$

$$\text{Put} \quad z_i = \begin{pmatrix} v_i \\ w_i \end{pmatrix}, \quad z_{i+q} = \begin{pmatrix} v_i \\ -w_i \end{pmatrix}$$

for $i = 1, \ldots, q$. The matrix Q whose columns are $z_1, \ldots, z_t$ reduces B to the Jondan canonical form.

Lemma 1.6. *Let B be a Hermitian matrix, $\begin{pmatrix} v \\ w \end{pmatrix}$, $\begin{pmatrix} v' \\ w' \end{pmatrix}$ two eigenvectors. Let*

$$\begin{pmatrix} v \\ w \end{pmatrix} \notin \mathscr{L}\left\{\begin{pmatrix} v' \\ w' \end{pmatrix}\right\}, \quad \begin{pmatrix} v \\ w \end{pmatrix} \notin \mathscr{L}\left\{\begin{pmatrix} v' \\ -w' \end{pmatrix}\right\}.$$

Then

$$v^{\mathrm{T}}v' = 0 \quad \textit{and} \quad w^{\mathrm{T}}w' = 0\,. \tag{23.6}$$

Proof. The statement follows immediately from the equations

$$\begin{pmatrix} v \\ w \end{pmatrix}^{\mathrm{T}}\begin{pmatrix} v' \\ w' \end{pmatrix} = 0 \quad \text{and} \quad \begin{pmatrix} v \\ w \end{pmatrix}^{\mathrm{T}}\begin{pmatrix} v' \\ -w' \end{pmatrix} = 0\,.$$ □

According to Theorem 2.6 the same can be evidently said for the eigenvectors of $\mathscr{L}_\omega$. For the matrix B we generally have only that $D^{1/2}BD^{-1/2}$ is a Hermitian matrix and therefore the orthogonality conditions (23.6) are not valid generally. The same is true for $\mathscr{L}_\omega$.

On the basis of these investigations the following assertion holds: If B is Hermitian then we have

$$\textit{Dominant quotient} = \max\left(\frac{\lambda_2(\omega)}{\lambda_1(\omega)}, \left(\frac{\lambda_3(\omega)}{\lambda_1(\omega)}\right)^2\right) \quad \text{for} \quad \omega \in \langle 1, \omega_2 \rangle\,. \tag{24.6}$$

In this case Assumption 2 is not valid but it is easy to calculate (2.3) and (3.3) directly using the orthogonal properties of eigenvectors which guarantee the validity of Theorem 1.3 and the subsequent theorems.

If the maximum in (24.6) equals $(\lambda_3(\omega)/\lambda_1(\omega))^2$ then we can put $q = \lambda_3(\omega)/\lambda_1(\omega)$, $\varkappa_2 = 2$ in Theorem 1.3 and the subsequent theorems. For $\varkappa_1$ we have $\varkappa_1 = 2$ if $\omega = \omega_2$ and $\varkappa_1 = 0$ if $\omega < \omega_2$. If the maximum in (2.4.6) equals $(\lambda_2(\omega)/\lambda_1(\omega))$ then $q = \lambda_2(\omega)/\lambda_1(\omega)$, $\varkappa_2 = 1$ and $\varkappa_1 = 0$.

If no orthogonal conditions hold, then

$$q = \frac{\lambda_3(\omega)}{\lambda_1(\omega)}, \quad \varkappa_2 = 1$$

and

$$\varkappa_1 = \begin{cases} 0 & \text{if} \quad \omega < \omega_2 \\ 1 & \text{if} \quad \omega = \omega_2 . \end{cases}$$

For the extrapolated vector $y_k = y_k(\omega)$ we have from Theorem 1.5

$$y_k - x^* = k^{\varkappa_1} \lambda_3^k(\omega) [w + u_k] ,$$

where $w \neq 0$ and

$$\{\|u_k\|\} = O\left(\frac{1}{k}\right) \quad \text{if} \quad \omega = \omega_2$$

and generally

$$\{\|u_k\|\} = O\left(\left(\frac{\lambda_3(\omega)}{\lambda_1(\omega)}\right)^k\right) \quad \text{if} \quad \omega < \omega_2 .$$

Our theory provides an algorithm based on Theorems 1.3–2.6 and relation (15.6) which minimizes $\lambda_3(\omega)$ in $(0, 2)$, and these together give an estimate for $\lambda_1(\omega_2)$, $\lambda_3(\omega_2)$, ω_1, ω_2. In the next section we give numerical results which show the advantages of our procedure.

7. NUMERICAL EXAMPLE

As an example we consider the numerical solution of the two-dimensional elliptic partial differential equation

$$-(D(x, y) u_x)_x - (D(x, y) u_y)_y + \sigma(x, y) u = S(x, y) ; \quad (x, y) \in R ,$$

where R is the square $0 < x, y < 2.1$, with the boundary condition $\partial u / \partial n = 0$, $(x, y) \in \Gamma$ where Γ is the boundary of R. The given functions D, σ and S are piecewise constant, with their values given in a Table (see [7] pp. 302–303, Appendix B). Using the method of integration based on a five point formula we derive the matrix equation $Au = 0$ because $S(x, y)$ was taken to be identically zero. Since the unique vector solution has zero components, the error in any vector iterate u_k arising from an iterative method of solving $Au = 0$ is just the vector itself. We solve the system by using S.O.R. method $u_{k+1} = \mathscr{L}_\omega u_k$. In Table 1 we compare the convergence of the approximations for ω_1 and ω_2 in dependence on k and ω. For the initial approximation we take the vector $u_0 = (1, 1, \ldots, 1)^T$. For a given number of iterations k we introduce the approximation for ω_1 and ω_2 in two rows which are denoted by $\omega_1(k)$ and $\omega_2(k)$.

The true value for ω_1 is 1·9177 (see [7] p. 304), for ω_2 we have obtained 1·514. In Table 2 we compare the numbers $y_k^T y_k$, where y_k are the extrapolated vectors, for various choices of the initial value of ω.

Table 1

k	$\omega\rightarrow$	1·5	1·45	1·40	1·35	1·25
12	$\omega_1(k)$	1·9184	1·9182	1·9165	1·9090	1·8552
	$\omega_2(k)$	1·5546	1·5048	1·4389	1·3850	1·2993
16	$\omega_1(k)$	1·9180	1·9182	1·9184	1·9186	1·9140
	$\omega_2(k)$	1·5167	1·5198	1·5049	1·4723	1·3995
18	$\omega_1(k)$	1·9178	1·9180	1·9182	1·9184	1·9177
	$\omega_2(k)$	1·5071	1·5137	1·5125	1·4911	1·4366
20	$\omega_1(k)$	1·9177	1·9178	1·9180	1·9182	1·9184
	$\omega_2(k)$	1·5142	1·5144	1·5151	1·5026	1·4568
26	$\omega_1(k)$	the same	the same	1·9177	1·9178	1·9180
	$\omega_2(k)$	the same	the same	1·5142	1·5139	1·4880
30	$\omega_1(k)$	the same	the same	the same	1·9177	1·9178
	$\omega_2(k)$	the same	the same	the same	1·5142	1·5074
40	$\omega_1(k)$	the same	the same	the same	the same	1·9177
	$\omega_2(k)$	the same	the same	the same	the same	1·5140

Table 2

$k \diagdown \omega$	1·5	1·45	1·40	1·35	1·25	1·0
12	$0{\cdot}424_{10^{-2}}$	$0{\cdot}120_{10^{-2}}$	$0{\cdot}153_{10^{-1}}$	$0{\cdot}550_{10^{0}}$	$0{\cdot}735_{10^{1}}$	$0{\cdot}153_{10^{2}}$
16	$0{\cdot}927_{10^{-2}}$	$0{\cdot}200_{10^{-2}}$	$0{\cdot}494_{10^{-2}}$	$0{\cdot}706_{10^{-2}}$	$0{\cdot}117_{10^{0}}$	$0{\cdot}131_{10^{2}}$
20	$0{\cdot}174_{10^{-4}}$	$0{\cdot}154_{10^{-3}}$	$0{\cdot}609_{10^{-3}}$	$0{\cdot}186_{10^{-2}}$	$0{\cdot}488_{10^{-2}}$	$0{\cdot}681_{10^{1}}$
24	$0{\cdot}263_{10^{-6}}$	$0{\cdot}877_{10^{-5}}$	$0{\cdot}568_{10^{-4}}$	$0{\cdot}235_{10^{-3}}$	$0{\cdot}219_{10^{-2}}$	$0{\cdot}117_{10^{1}}$
28	$0{\cdot}416_{10^{-8}}$	$0{\cdot}467_{10^{-6}}$	$0{\cdot}508_{10^{-5}}$	$0{\cdot}218_{10^{-4}}$	$0{\cdot}423_{10^{-3}}$	$0{\cdot}430_{10^{-1}}$

Table 3

k	Optimal extrapol. S.O.R.	Optimal S.O.R.
12	$0{\cdot}613_{10^{-2}}$	$0{\cdot}843_{10^{1}}$
16	$0{\cdot}834_{10^{-3}}$	$0{\cdot}579_{10^{1}}$
20	$0{\cdot}620_{10^{-5}}$	$0{\cdot}383_{10^{1}}$
24	$0{\cdot}290_{10^{-7}}$	$0{\cdot}306_{10^{1}}$

In Table 3 we compare numbers $y_k^T y_k$ of the optimal extrapolated S.O.R. (i.e. $\omega \doteq \omega_2 \doteq 1.5142$) with the numbers $u_k^T u_k$ of the optimal S.O.R. ($\omega = 1.9177$).

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Souhrn

DVOUKROKOVÁ EXTRAPOLACE A OPTIMÁLNÍ VÝBĚR RELAXAČNÍHO FAKTORU EXTRAPOLOVANÉ METODY S.O.R.

JAN ZÍTKO

Limity extrapolačních koeficientů jsou racionální funkce několika pólů o největší absolutní hodnotě rezolventy $R(\lambda, T) = (\lambda I - T)^{-1}$. Dobrý odhad těchto pólů může býti vypočítán z těchto koeficientů. Výpočet je velmi snadný v případě dvou koeficientů a zejména v konečně rozměrných prostorech je možné využít těchto poznatků k urychlení konvergence při řešení soustav lineárních algebraických rovnic metodou S.O.R. Numerické výsledky uvedené na konci práce ukazují efektivitu extrapolované metody S.O.R.

Резюме

ДВУХШАГОВАЯ ЭКСТРАПОЛЯЦИЯ И ОПТИМАЛЬНАЯ ВЫБОРКА РЕЛАКСАЦИОННОГО ФАКТОРА ЭКСТРАПОЛИРОВАННОГО МЕТОДА S.O.R.

JAN ZÍTKO

Пределы экстраполяционных коэффициентов являются рациональными функциями нескольких максимальных по модулю полюсов резольвентного оператора $R(\lambda, T) = (\lambda I - T)^{-1}$. Поэтому из экстраполяционных коэффициентов можно получить хорошие оценки этих полюсов. Вычисление особенно просто в случае двух коэффициентов. Эти факты можно использовать например в конечномерных пространствах при решении линейных систем методом верхней релаксации. Численные результаты в конце работы демострируют эффективность экстраполированного метода S.O.R.

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