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Abstract

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ON AN ACCELERATED "REFINEMENT OF THE ROOTS OF SECULAR EQUATIONS" BY THE MAYANTS METHOD

(Presented by Academician I. V. Obreimov, March 4, 1959)

By the method of Mayants ([1]), the roots λ of the secular equation

$$|W - \lambda K| = 0, \tag{1}$$

where

$$W = \|w_{ij}\|_n^n, \qquad K = \|k_{ij}\|_n^n,$$

and the corresponding solutions

$$X = \begin{Vmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{Vmatrix}$$

of the system of homogeneous linear equations

$$(W - \lambda K)X = 0 \tag{2}$$

are obtained as the limits of convergent sequences $\{\lambda_{(s)}\}$ and $\{X_{(s)}\}$, formed under iteration with the aid of the relations

$$\lambda_{(1)} = \lambda_0; \tag{3}$$

$$X'_{(s)} = -B_{(s)}^{-1} V_{(s)}; \tag{4}$$

$$\lambda_{(s+1)} = \frac{w_{11} + V'_{(s)} X'_{(s)} - \lambda_{(s)} \left[V'_{(s)} (\partial X' / \partial \lambda)_{(s)} - K'_1 X'_{(s)} \right]}{k_{11} - \left[V'_{(s)} (\partial X' / \partial \lambda)_s - K'_1 X'_{(s)} \right]}, \tag{5}$$

where $B_{(s)} = W' - \lambda_{(s)} K'$ is a matrix of order $(n-1)$ with elements $b_{ij} = w_{ij} - \lambda_{(s)} k_{ij}$ $(i, j \neq 1)$;

$$X'_{(s)} = \begin{Vmatrix} x_2 \\ x_3 \\ \vdots \\ x_n \end{Vmatrix}, \qquad X_{(s)} = \begin{Vmatrix} 1 \\ \cdots \\ X'_{(s)} \end{Vmatrix};$$

$$V_{(s)} = W_1 - \lambda_{(s)} K_1, \qquad W_1 = \begin{Vmatrix} w_{21} \\ w_{31} \\ \vdots \\ w_{n1} \end{Vmatrix}, \qquad K_1 = \begin{Vmatrix} k_{21} \\ k_{31} \\ \vdots \\ k_{n1} \end{Vmatrix};$$

$$V'_{(s)} = W'_1 - \lambda_{(s)} K'_1, \qquad W'_1 = \| w_{12}, w_{13}, \dots, w_{1n} \|, \qquad K'_1 = \| k_{12}, k_{13}, \dots, k_{1n} \|.$$

If

$$\lambda_{(q)} = \frac{w_{11} + V_{(q)} X'_{(q)}}{k_{11}},$$

then (to the accuracy of the calculation) the true root of the secular equation (1) is

$$\lambda_{(\infty)} = \lambda_{(q)}.$$

and the corresponding solution of system (2)

$$X_{(\infty)} = X_{(q)}.$$

In the present paper it is shown that, in Mayants' computational scheme [1], at any iteration stage $s = s_0$ one can construct the power series

$$X'_{(t)} = X'_{(s_0)} + \sum_{n=1}^{\infty} \frac{1}{n!} \left(\frac{\partial^n X'}{\partial \lambda^n} \right)_{(s_0)} \left(\lambda_{(t)} - \lambda_{(s_0)} \right)^n \tag{6}$$

for the function $X'_{(t)}$, defined by relation (4), and, with the aid of this series, if it converges absolutely, accelerate the realization of the iterative process.

Indeed, from (4) it follows that

$$\left(\frac{\partial^n X'}{\partial \lambda^n} \right)_{(s_0)} = n! \left(B^{-1}_{(s_0)} K' \right)^{n-1} B^{-1}_{(s_0)} \left(K' X_{(s_0)} + K_1 \right). \tag{7}$$

Substituting (7) into (6), we obtain

$$X'_{(t)} = X'_{(s_0)} + \sum_{n=1}^{\infty} \left(B^{-1}_{(s_0)} K'\right)^{n-1} B_{(s_0)} (K' X'_{(s_0)} + K_1) \left(\lambda_{(t)} - \lambda_{(s_0)}\right)^{n}. \quad (8)$$

The coefficients of series (8), A_n $(n = 2, 3, ...)$, satisfy the recurrence relation

$$A_n = B^{-1}_{(s_0)} K' A_{n-1} \quad \text{for} \quad A_1 = B^{-1}_{(s_0)} (K' X'_{(s_0)} + K_1), \quad (9)$$

from which it follows that A_n can be computed successively at the s_0-th iteration stage, carrying out additional "convolutions" and constructing solutions of "chains" [(1)] for the columns of the free terms $K'A_1$, $K'A_2, ...$ If series (8) converges absolutely, then it satisfies the relation*

$$B_{(t)} X'_{(t)} = -V_{(t)}$$

and therefore can be used for approximation to $X'_{(\infty)}$. Indeed, from the absolute convergence of series (8) follows the absolute convergence of the series

$$\left(\frac{\partial X'}{\partial \lambda}\right)_{(t)} = \sum_{n=1}^{\infty} n \left(B^{-1}_{(s_0)} K'\right)^{n-1} B^{-1}_{(s_0)} (K' X'_{(s_0)} + K_1) \left(\lambda_{(t)} - \lambda_{(s_0)}\right)^{n-1}. \quad (10)$$

Series (8) and (10) make it possible to find $\lambda_{(t+1)}$ from (5). The same series (8) and (10) lead to $X'_{(t+1)}$ and $(\partial X'/\partial\lambda)_{(t+1)}$, after which $\lambda_{(t+2)}$, etc., is again determined from (5).

Alongside (2), by the indicated method one can solve system (11) for the transposed matrices $\widetilde{W}$ and $\widetilde{K}$:

$$(\widetilde{W} - \lambda_{(\infty)} \widetilde{K}) P = 0, \quad (11)$$

where

$$P = \begin{Vmatrix} p_1 \\ p_2 \\ \vdots \\ p_n \end{Vmatrix}, \quad \text{and, if } p_1 = 1 \text{ and } P' = \begin{Vmatrix} p_2 \\ p_3 \\ \vdots \\ p_n \end{Vmatrix}, \quad \text{then}$$

$$P'_{(s)} = -\widetilde{B}^{-1}_{(s)} \widetilde{V}'_{(s)}. \quad (12)$$

As shown in paper [2], the solution of (12) of the system $\widetilde{B}_{(s)}P'_{(s)} = -\widetilde{V}'_{(s)}$ is easily obtained in the same computational scheme, if the solution (4) has been constructed

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* This is easy to verify by substituting into the left-hand side of the given equality (8) and (15).

Table 1

III				IV(Computations relating to the solution of system (11) (?))								
$-\widetilde{B}^{-2}_{(s_0)}P'_{(s_0)}$;	0,130	1,213										
$-\widetilde{B}^{-1}_{(s_0)}P'_{(s_0)}$;	−0,811	−0,718										
$-P_{(s_0)}$;	−0,280	0,632										
$\Delta_{(s_0)}$ = 0,400;	0,782	−0,276	W_1 W'_1;	$-X'_{(s_0)}$	$-\widetilde{B}^{-1}_{(s_0)}X'_{(s_0)}$	$-\widetilde{B}^{-2}_{(s_0)}X'_{(s_0)}$	$-\widetilde{B}^{-3}_{(s_0)}X'_{(s_0)}$	$X'_{(s_0)}$				
	0,967 1;	−0,284	−0,374	−0,134	−0,389	0,062	−0,523	0,290	0,782 0,632	0,839 −0,718	−0,134 −0,811	1,126 −0,130
	*	−0,273	−0,362	−0,130	−0,376	0,060	−0,506					
	−0,779	−0,561	−0,365	0,836	−0,950	1,606	−2,136				1,213	−1,612
	0,255	−0,843	−0,739	0,702	−1,339	1,668	−2,659					II
	−1,292	−0,774	−0,647	0,735	−1,243	−1,653	−2,530		|0,489|	|−0,556|	|0,939|	|−1,248|
	*		0,836	−0,950	1,606	2,136	3,269					I
$\Delta_{(s_0+1)}$ = 0,224; $X'_{(s_0)}$;	0,134	−0,836	0,126				0,126	0,280	−0,632			$P'_{(s_0)}$
$\widetilde{B}^{-1}_{(s_0)}X'_{(s_0)}$;	0,389	0,950	−0,566	−0,176		−0,164	−0,565	0,811	0,718			$\widetilde{B}^{-1}_{(s_0)}P'_{(s_0)}$
$\widetilde{B}^{-2}_{(s_0)}X'_{(s_0)}$;	0,062	−1,606	0,492	0,031	−0,352	0,026	0,491	−0,130	−1,213			$\widetilde{B}^{-2}_{(s_0)}P'_{(s_0)}$
$\widetilde{B}^{-3}_{(s_0)}X'_{(s_0)}$;	0,523	2,136	−0,998	−0,005	0,093	−0,004	−0,996	1,089	1,612			$\widetilde{B}^{-3}_{(s_0)}P'_{(s_0)}$
$\widetilde{B}^{-4}_{(s_0)}X'_{(s_0)}$;	0,386	−3,269		0,001	−0,020	0,001	0,236	0,140	−0,789			$P'_{(s_0+2)} = P'_{(\infty)}$

III				IV (Computations relating to the solution of system (11) (?))			
$\Delta_{(s_0=2)} =$ 0,236; $X'_{(s_0+1)}$;	0,061	−1,067	0,247	$(\Delta_{(s_0+1)} - \Delta_{(s_0)})^n$	$n(\Delta_{(s_0+1)} - \Delta_{(s_0)})^{n-1}$	$(\Delta_{(s_0+2)} - \Delta_{(s_0)})^n$;	$\widetilde{W}_1 \widetilde{B}^{-n}_{(t)} P'_{(t)}$
$(\partial X'/\partial\lambda)_{(s_0+1)}$;	0,456	1,779	−0,848	−0,164	0,012		
$X'_{(\infty)} = X'_{(s_0+2)}$;	0,066	−1,044	0,237	$\Delta_{(s_0+2)} - \Delta_{(s_0)}$;	$\Delta_{(s_0+2)} - \Delta_{(s_0+1)}$		
$\Delta_{(\infty)} = \Delta_{(s_0+2)}$;			$W'_1 \widetilde{B}^{-n}_{(t)} X'_{(t)}$	$\Delta_{(s_0)}$; $\Delta_{(s_0+1)}$			

Notes. 1. The headings in the columns enclosed between lines III and IV refer to the numbers located above line II, not counting the numbers situated in the row marked with an asterisk. 2. In computing the coefficients of series (14′), the check formula $\widetilde{W}_1 \widetilde{B}^{-n}_{(t)} P'_{(t)} = \widetilde{B}^{-n}_{(t)} X'_{(t)} \widetilde{W}'_1 = \widetilde{W}'_1 \widetilde{B}^{-n}_{(t)} X'_{(t)}$ was used.

system $B_{(s)} X_{(s)} = -V_{(s)}$. Replacing in (8): $X'_{(t)}$ by $P'_{(t)}$; $X'_{(s_0)}$ by $P'_{(s_0)}$; $B^{-1}_{(s_0)}$ by $\widetilde{B}^{-1}_{(s_0)}$; K' by $\widetilde{K}'$ and K_1 by $\widetilde{K}_1$, we obtain

$$P'_{(t)} = P'_{(s_0)} + \sum_{n=1}^{\infty} (\widetilde{B}^{-1}_{(s_0)} \widetilde{K}')^{n-1} \widetilde{B}^{-1}_{(s_0)} (\widetilde{K}' P'_{(s_0)} + \widetilde{K}_1)(\lambda_{(t)} - \lambda_{(s_0)})^n. \qquad (13)$$

The coefficients of series (13), $A'_n = \widetilde{B}^{-1}_{(s_0)} \widetilde{K}' A_{n-1}$ $(n = 2, 3, ...)$, are determined, with $A'_1 = \widetilde{B}^{-1}_{(s_0)} (\widetilde{K}' P'_{(s_0)} + \widetilde{K}_1)$, by relations of type (12) and, consequently, can be computed in the same way as $P'_{(s_0)}$. Substituting $\lambda_{(t)} = \lambda_{(\infty)}$ in (13), we obtain

$$P'_{(\infty)} = P'_{(s_0)} + \sum_{n=1}^{\infty} (\widetilde{B}^{-1}_{(s_0)} \widetilde{K}')^{n-1} B^{-1}_{(s_0)} (\widetilde{K}' P'_{(s_0)} + K'_1)(\lambda_{(\infty)} - \lambda_{(s_0)})^n. \qquad (14)$$

Thus, the absolute convergence of series (8) makes it possible to perform $q - s_0$ iterations within the framework of the s_0-th computation step, without solving $q - s_0$ systems $BX'_{(t)} = -V_{(t)}$ $(t = s_0 + 1, s_0 + 2, \ldots, q)$, and to find $\lambda_{(\infty)}$, $X'_{(\infty)}$, and $P'_{(\infty)}$. The use of series (8) and (10) instead of (4), and of series (14) instead of $P'_{(\infty)} = -\widetilde{B}^{-1}_{(\infty)}\widetilde{V}'_{(\infty)}$, leads to an accelerated "refinement of the roots of secular equations."

In the most practically important case $K = E$ $(K' = E)$, relations (8), (10), (5), and (14) are transformed respectively into

$$X'_{(t)} = X'_{(s_0)} + \sum_{n=1}^{\infty} B^{-n}_{(s_0)} X'_{(s_0)} (\Delta_{(t)} - \Delta_{(s_0)})^n, \tag{8'}$$

where $\Delta_{(s)} = \lambda_{(s)} - w_{11}$;

$$\left(\frac{\partial X'}{\partial \Delta}\right)_{(t)} = \sum_{n=1}^{\infty} n B^{-n}_{(s_0)} X'_{(s_0)} (\Delta_{(t)} - \Delta_{(s_0)})^{n-1}, \tag{10'}$$

$$\Delta_{(s+1)} = \frac{W'_1 X'_{(s)} - \Delta_{(s)} W'_1 (\partial X'/\partial \Delta)_{(s)}}{1 - W'_1 (\partial X/\partial \Delta)_{(s)}}; \tag{5'}$$

$$P'_{(\infty)} = P'_{(s_0)} + \sum_{n=1}^{\infty} \widetilde{B}^{-n}_{(s_0)} P'_{(s_0)} (\Delta_{(\infty)} - \Delta_{(s_0)})^n, \tag{14'}$$

where

$$P'_{(s_0)} = -\widetilde{B}^{-1}_{(s_0)} \widetilde{W}'_1. \tag{12'}$$

Table 1 gives the computation for the case $K = E$, carried out according to the scheme of accelerated "root refinement." *

The method of iteration with the aid of a power series is worth applying in the case when the number of additional operations $B^{-1}K'A_n$, required (within the accuracy of the computation) for the equivalent replacement of relation (4) by series (8),** is small.

In conclusion, I express my gratitude to L. S. Mayants and I. V. Obreimov for discussing the results and for their interest in the work.

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References

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2. L. S. Mayants, *Optics and Spectroscopy*, **5**, 378 (1958).

* This scheme is based on the computational scheme of Mayants (1).

** Moreover, for the equivalent replacement of the relation

$$(\partial X'/\partial\lambda)_{(s)} = +B_{(s)}^{-1}(K'X'_{(s)}K_1)$$

by series (10).

Note: Figure translations are in progress. See original paper for figures.