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INVERSE EIGENVALUE PROBLEM FOR PERIODIC BLOCK JACOBI MATRICES

1. Introduction. In this paper we consider an inverse eigenvalue problem for periodic block Jacobi matrices (PBJ matrices). It is the extended problem of constructing a periodic Jacobi matrix (see, e.g., [2]). To compute such a matrix we apply Lanczos' algorithm. The aim of this paper is to define conditions which are sufficient to construct a PBJ matrix and to formulate an algorithm of computing this matrix. The algorithm is based on some modification of Lanczos' algorithm (see [2], [5], and [4]).

Now we introduce some notation and the definition of a PBJ matrix.

Definition. A real symmetric matrix $T = (t_{ij})_{i,j=1}^{n}$ is called a *periodic block Jacobi matrix* if it has the block representation

$$T = \begin{vmatrix} M_1 & R_1^T & & R_p \\ R_1 & \ddots & \ddots & \\ & \ddots & \ddots & R_{p-1}^T \\ R_p^T & & R_{p-1} & M_p \end{vmatrix},$$

where M_i are symmetric $(r\times r)$-matrices, and R_i are upper triangular $(r\times r)$-matrices, $rp = n$.

The matrix obtained from the matrix T by striking the first K columns and rows is denoted by $T^{(K)}$. The matrix which differs from $T^{(K)}$ only in signs of the elements $t_{K+1,n-r+K+1}$ and $t_{n-r+K+1,K+1}$ is denoted by $T_-^{(K)}$. Note that $T^{(K)} = (t_{ij})_{i,j=K+1}^{n}$.

Let $\{\mu_i^{(K)}\}_{i=1}^{n-K}$ $(K = 0, \ldots, r)$ be the eigenvalues of the matrix $T^{(K)}$ and let $\{\nu_i^{(K)}\}_{i=1}^{n-K}$ $(K = 0, \ldots, r-1)$ be the eigenvalues of the matrix $T_-^{(K)}$.

By $Q^{(K)}$ we denote the orthogonal matrix whose columns are eigenvectors of $T^{(K)}$. Let the columns of $Q^{(K)T}$ be denoted by $p_j^{(K)}$:

$$Q^{(K)} = [p_1^{(K)}, \ldots, p_{n-K}^{(K)}]^T.$$

We consider also matrices $L^{(K)}$ and $L_-^{(K)}$ formed in the following way:

$$L^{(K)} = \begin{vmatrix} t_{K+1,K+1} & \hat{b}^{(K)T} \\ \hat{b}^{(K)} & M^{(K)} \end{vmatrix} = \begin{vmatrix} 1 & \emptyset^T \\ \emptyset & Q^{(K+1)T} \end{vmatrix} T^{(K)} \begin{vmatrix} 1 & \emptyset^T \\ \emptyset & Q^{(K+1)} \end{vmatrix},$$

$$L_-^{(K)} = \begin{vmatrix} t_{K+1,K+1} & \tilde{b}^{(K)T} \\ \tilde{b}^{(K)} & M^{(K)} \end{vmatrix} = \begin{vmatrix} 1 & \emptyset^T \\ \emptyset & Q^{(K+1)T} \end{vmatrix} T_-^{(K)} \begin{vmatrix} 1 & \emptyset^T \\ \emptyset & Q^{(K+1)} \end{vmatrix}.$$

where $M^{(K)} = \operatorname{diag}(\mu_i^{(K+1)})$, $\emptyset$, $\tilde{b}^{(K)}$, $\hat{b}^{(K)} \in R^{n-K-1}$.

Now we formulate the inverse eigenvalue problem for the PBJ matrix.

Assume that for given sequences $\{\mu_i^{(K)}\}_{i=1}^{n-K}$ $(K = 0, \ldots, r)$ and $\{\nu_i^{(K)}\}_{i=1}^{n-K}$ $(K = 0, \ldots, r-1)$ the following strong interlace conditions hold:

(i) $\mu_i^{(K)} < \mu_i^{(K+1)} < \mu_{i+1}^{(K)}$ $(K = 0, \ldots, r-1;\ i = 1, \ldots, n-K-1)$,

(ii) $\nu_i^{(K)} < \nu_i^{(K+1)} < \nu_{i+1}^{(K)}$ $(K = 0, \ldots, r-1;\ i = 1, \ldots, n-K-1)$.

Then we want to find a PBJ matrix T of order n such that

(iii) $\operatorname{sp}(T^{(K)}) = \{\mu_i^{(K)}\}_{i=1}^{n-K}$ $(K = 0, \ldots, r)$,

(iv) $\operatorname{sp}(T_-^{(K)}) = \{\nu_i^{(K)}\}_{i=1}^{n-K}$ $(K = 0, \ldots, r-1)$.

In Section 2 we present Lanczos' algorithm and we show how it may be applied to the construction of a PBJ matrix. Before applying Lanczos' algorithm one should compute some coordinates of the orthonormal eigenvectors of the matrix T. To this end, in Section 3 we give formulas for these values and finally we formulate the algorithm of computing a PBJ matrix.

2. Lanczos' algorithm. Now we describe Lanczos' algorithm which in some special cases yields PBJ matrices.

Let A be a real symmetric matrix of order n and let r be an integer such that $rp = n$ for some $p \in N$. Let U_0 and U_1 be matrices of size $n \times r$ such that $U_i^T U_j = 0$ $(i \neq j,\ i, j = 0, 1)$, $U_i^T U_i = I$ $(i = 0, 1)$, $U_1^T A U_0$ is an upper triangular, nonsingular matrix. We form the sequence of matrices $U_2, \ldots, U_p, M_1, \ldots, M_p, R_1, \ldots, R_p$ as follows:

(a) $R_0 \equiv R_p = U_1^T A U_0$,

(b) $M_p = U_0^T A U_0$,

(c) $M_i = U_i^T A U_i$ $(i = 1, \ldots, p-1)$,

(d) $D_i = AU_i - U_i M_i - U_{i-1} R_{i-1}^T$ $(i = 1, \ldots, p-1)$,

(e) $D_i \equiv U_{i+1} R_i$ $(i = 1, \ldots, p-1)$.

Remarks. 1. In the block Lanczos' algorithm (see [1]), $U_0 \equiv 0$.

2. The identity (e) denotes QR factorization of the full-rank matrix D_i. We assume that positive diagonal elements are chosen in R_i. If D_i is rank-deficient, then the algorithm fails.

THEOREM. *If the symmetric $(n \times n)$-matrix A $(n = rp$, where r and p are natural$)$ is orthogonally similar to the matrix T of the PBJ form*

$$U^T AU = T = \begin{vmatrix} M_1 & R_1^T & & R_p \\ R_1 & \ddots & \ddots & \\ & \ddots & \ddots & R_{p-1}^T \\ R_p^T & & R_{p-1} & M_p \end{vmatrix}, \quad U^T U = I,\ U = [U_1, \ldots, U_p],$$

with nonsingular upper triangular blocks $R_1, \ldots, R_p$ *having positive elements on the diagonals in* $R_1, \ldots, R_{p-1}$, *then the Lanczos algorithm* (a)–(e) *starting with* $U_0 = U_p$ *and* U_1 *determines* $\{M_i, R_i\}_{i=1}^p$ *and* $\{U_i\}_{i=2}^p$.

Proof. Since $AU = UT$, it is easy to verify that with the notation $R_0 \equiv R_p$, $U_1 \equiv U_{p+1}$ and $U_0 \equiv U_p$ we obtain

$$AU_i = U_{i-1} R_{i-1}^T + U_i M_i + U_{i+1} R_i \quad (i = 1, \ldots, p).$$

Hence, by the orthogonality of the matrix U,

$$U_i^T AU_i = M_i \quad (i = 1, \ldots, p),$$

and also

$$D_i \equiv U_{i+1} R_i = AU_i - U_i M_i - U_{i-1} R_{i-1}^T \quad (i = 1, \ldots, p).$$

This completes the proof because D_i has a unique decomposition into a product of a matrix having orthogonal columns and an upper triangular matrix having positive elements on the main diagonal.

Remark. One can show that to determine the PBJ matrix T it is sufficient to know any two consecutive matrices U_{i-1} and U_i. In this case

$$U_{K+1} R_K = AU_K - U_K M_K - U_{K-1} R_{K-1}^T \quad (K = i, \ldots, i+p-1)$$

with initial values $M_i = U_i^T AU_i$ and $R_{i-1} = U_i^T AU_{i-1}$, using periodic indexing

$$U_K \equiv U_{K-p}, \quad M_K \equiv M_{K-p}, \quad R_K \equiv R_{K-p} \quad \text{for } K \geqslant p.$$

Thus, the knowledge of U_0 and U_1 is a sufficient condition (not necessary) for the construction of the matrix T.

From the above considerations it follows that to solve the inverse eigenvalue problem for a PBJ matrix by Lanczos' algorithm it is sufficient to compute the first and last r rows of the matrix $Q^{(0)}$. In other words: if we know the vectors $p_1^{(0)}, \ldots, p_r^{(0)}$ and $p_{n-r+1}^{(0)}, \ldots, p_n^{(0)}$, then we can compute the matrix T taking

$$A = \mathrm{diag}(\mu_i^{(0)}), \quad U_0 = [p_{n-r+1}^{(0)}, \ldots, p_n^{(0)}], \quad U_1 = [p_1^{(0)}, \ldots, p_r^{(0)}],$$

and performing the Lanczos algorithm (a)–(e).

3. Construction of a Jacobi matrix. Now we discuss the way in which we compute the vectors $p_1^{(0)}, \ldots, p_r^{(0)}$ and $p_{n-r+1}^{(0)}, \ldots, p_n^{(0)}$ and formulate the algorithm solving the inverse eigenvalue problem.

Golub [3] gave some relationship among the eigenvalues of a symmetric matrix, the eigenvalues of its right principal submatrix, and the vector of first coordinates of the orthonormal eigenvectors of this matrix. In our notation this relationship has the form

$$(1)\qquad p_{1,i}^{(K)2} = \frac{\prod_{j=1}^{n-K-1} (\mu_j^{(K+1)} - \mu_i^{(K)})}{\prod_{\substack{j=1\\ j\neq i}}^{n-K} (\mu_j^{(K)} - \mu_i^{(K)})} \qquad (i = 1, \ldots, n-K).$$

Formula (1) enables us to compute the vectors $p_1^{(K)}$ $(K = 0, \ldots, r-1)$ because from the interleaving condition (i) it follows that the right-hand side of (1) is positive. Moreover, we can pick the signs of $p_{1,i}^{(K)}$ arbitrarily, since changing one sign is equivalent to multiplying the corresponding eigenvector by -1.

Now we determine the vectors $p_{n-r}^{(K)}$, $(K = 1, \ldots, r)$. To this end we consider the characteristic polynomials of matrices $L^{(K)}$ and $L_-^{(K)}$. It is easy to check that

$$\mathrm{sp}(L^{(K)}) = \{\mu_i^{(K)}\}_{i=1}^{n-K},$$

whence

$$\det(L^{(K)} - tI) = \prod_{i=1}^{n-K} (\mu_i^{(K)} - t).$$

The form of the matrix $L^{(K)}$ may be used to prove that

$$\det(L^{(K)} - tI)$$
$$= (t_{K+1,K+1} - t) \prod_{i=1}^{n-K-1} (\mu_i^{(K+1)} - t) - \sum_{j=1}^{n-K-1} \hat{b}_j^{(K)2} \prod_{\substack{i=1\\ i\neq j}}^{n-K-1} (\mu_i^{(K+1)} - t).$$

Equating both above expressions for $t = \mu_i^{(K+1)}$ we obtain

$$(2)\qquad \hat{b}_i^{(K)2} = -\prod_{j=1}^{n-K} (\mu_j^{(K)} - \mu_i^{(K+1)}) \Big/ \prod_{\substack{j=1\\ j\neq i}}^{n-K-1} (\mu_j^{(K+1)} - \mu_i^{(K+1)})$$

and, analogously for the matrix $L_-^{(K)}$,

$$(3)\qquad \tilde{b}_i^{(K)2} = -\prod_{j=1}^{n-K} (\nu_j^{(K)} - \nu_i^{(K+1)}) \Big/ \prod_{\substack{j=1\\ j\neq i}}^{n-K-1} (\nu_j^{(K+1)} - \nu_i^{(K+1)}).$$

Notice that the right-hand sides of (2) and (3) are positive. This follows from conditions (i) and (ii). The numerators of the right-hand sides have $i-1$ negative factors each, and the denominators have i such factors each. Thus $-\hat{b}_i^{(K)2}$ and $-\tilde{b}_i^{(K)2}$ are negative.

Subtracting $L_-^{(K)}$ from $L^{(K)}$ we obtain

$$\hat{b}^{(K)} - \tilde{b}^{(K)} = 2t_{K+1,n-r+K+1}\, p_{n-r}^{(K+1)}.$$

But $\|p_{n-r}^{(K+1)}\|_2 = 1$, so

$$p_{n-r}^{(K+1)} = (\hat{b}^{(K)} - \tilde{b}^{(K)})/\|\hat{b}^{(K)} - \tilde{b}^{(K)}\|. \tag{4}$$

Formula (4) is properly defined since the nonsingularity of the upper triangular matrix R_p guarantees that $\hat{b}^{(K)} \neq \tilde{b}^{(K)}$. Notice also that with different combinations of the signs of the elements $\tilde{b}_i^{(K)}$ and $\hat{b}_i^{(K)}$ there are generally associated different values of the vectors $p_{n-r}^{(K+1)}$. It is thus necessary to verify all combinations of sign changes.

Boley and Golub ([1], [2]) proved that

$$p_{j,i}^{(K)} = -p_{1,i}^{(K)} \sum_{m=1}^{n-K-1} \left(p_{j-1,m}^{(K+1)}\, \hat{b}_m^{(K)}/(\mu_m^{(K+1)} - \mu_i^{(K)})\right). \tag{5}$$

This means that if we know the vectors $p_1^{(K)}$, $p_{j-1}^{(K)}$ and $\hat{b}^{(K)}$, then we can compute the vector $p_j^{(K)}$. Let us remember that $p_1^{(K)}$ may by computed from (1), and $\hat{b}^{(K)}$ from (2). Thus all necessary vectors may be determined by applying formula (5) repeatedly.

This procedure is illustrated by the following scheme:

$$\begin{array}{r}
p_{n-r}^{(r)} \to p_{n-r+1}^{(r-1)} \to p_{n-r+2}^{(r-2)} \to \dots \to p_{n-1}^{(1)} \to p_n^{(0)} \\
p_{n-r}^{(r-1)} \to p_{n-r+1}^{(r-2)} \to \dots \to p_{n-2}^{(1)} \to p_{n-1}^{(0)} \\
p_{n-r}^{(r-2)} \to \dots \to p_{n-3}^{(1)} \to p_{n-2}^{(0)} \\
\dots\dots\dots\dots\dots\dots \\
\dots\ p_{n-r+1}^{(1)} \to p_{n-r+2}^{(0)} \\
p_{n-r}^{(1)} \to p_{n-r+1}^{(0)} \\
p_1^{(r-1)} \to p_2^{(r-2)} \to \dots \to p_{r-1}^{(1)} \to p_r^{(0)} \\
p_1^{(r-2)} \to \dots \to p_{r-2}^{(1)} \to p_{r-1}^{(0)} \\
\dots\ p_{r-3}^{(1)} \to p_{r-2}^{(0)} \\
\dots\dots\dots \\
p_1^{(1)} \to p_2^{(0)} \\
\to p_1^{(0)}.
\end{array}$$

Last of all we give the complete algorithm of the inverse eigenvalue problem for a PBJ matrix.

ALGORITHM.

Data: $\{\mu_i^{(K)}\}_{i=1}^{n-K}$ $(K = 0, \dots, r)$, $\{\nu_i^{(K)}\}_{i=1}^{n-K}$ $(K = 0, \dots, r-1)$.

Step I. We compute the vectors $p_1^{(0)}, \ldots, p_r^{(0)}$ and $p_{n-r+1}^{(0)}, \ldots, p_n^{(0)}$ in the following way: for $j = 1, \ldots, r$

compute $\hat{b}^{(r-j)}$ from (2),

compute $p_1^{(r-j)}$ from (1),

compute $p_{n-r}^{(r-j+1)}$ from (3) and (4),

compute $p_i^{(r-j-i+1)}$ from (5) $(i = 2, \ldots, r-j+1)$,

compute $p_{n+i-r}^{(r-j-i+1)}$ from (5) $(i = 1, \ldots, r-j+1)$.

While computing with the use of formulas (2) and (3) one should keep in mind the necessity of verifying all sign combinations. Thus the Lanczos algorithm guarantees only essential constructibility of the PBJ matrix.

Step II. Using Lanczos' algorithm we determine the matrices $U_2, \ldots, U_p$, $M_1, \ldots, M_p$, $R_1, \ldots, R_p$ (formulas (1)–(5)) taking

$$U_0 = [p_{n-r+1}^{(0)}, \ldots, p_n^{(0)}], \quad U_1 = [p_1^{(0)}, \ldots, p_r^{(0)}], \quad A := \operatorname{diag}(\mu_i^{(0)}).$$

Then the matrix T determined by the Theorem is a PBJ matrix which solves the above formulated eigenproblem.

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