MATHEMATICS OF COMPUTATION
VOLUME 42, NUMBER 165
JANUARY 1984, PAGES 143-150

A Modified Method for Reconstructing Periodic Jacobi Matrices

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Abstract. In this note, we discuss the reconstruction of periodic Jacobi matrices from spectral data. The method combines ideas and techniques from the algorithms given by Boley and Golub [1], [2], and Ferguson [3], resulting in a numerically stable algorithm applicable to a larger class of problems. The number of initial data items needed for this method equals the number of items in the resulting matrix, namely $2n$.

1. Introduction. In this note, we discuss the reconstruction of a periodic Jacobi matrix of the form

$$J = \begin{bmatrix} a_1 & b_1 & & & & & b_n \\ b_1 & a_2 & \cdot & & & & \\ & \cdot & \cdot & \cdot & & 0 & \\ & & \cdot & \cdot & \cdot & & \\ & 0 & & \cdot & \cdot & \cdot & \\ & & & & \cdot & a_{n-1} & b_{n-1} \\ b_n & & & & & b_{n-1} & a_n \end{bmatrix} \tag{1a}$$

from the eigenvalue data using methods that are numerically stable. Here the a_i and b_i are real, and $b_i \neq 0$ for all i. Such problems arise, for example, in the study of Toda Lattices [9], [10], and might also arise in the study of Sturm-Liouville and Hill's equations [3]. In particular, we are given the following initial information: the eigenvalues λ_i, $i = 1,\ldots, n$ of J, the eigenvalues μ_i, $i = 1,\ldots, n-1$ of the submatrix $\bar{J}$ obtained from J by deleting the first row and column. We also need the product $\beta = b_1 b_2 \cdots b_n$, or equivalently the eigenvalues λ_i^-, $i = 1,\ldots, n$ of the matrix

$$J^- = \begin{bmatrix} a_1 & b_1 & & & & & -b_n \\ b_1 & a_2 & \cdot & & & & \\ & \cdot & \cdot & \cdot & & 0 & \\ & & \cdot & \cdot & \cdot & & \\ & 0 & & \cdot & \cdot & \cdot & \\ & & & & \cdot & a_{n-1} & b_{n-1} \\ -b_n & & & & & b_{n-1} & a_n \end{bmatrix} \tag{1b}$$

Received October 5, 1982.
1980 *Mathematics Subject Classification*. Primary 15A18, 65F15.
*We gratefully acknowledge the support of the National Science Foundation under grant ECS-8204468 for the first author and the Department of Energy under grant DE-AT03-76ER 71030 for the second author.

0025-5718/84 $1.00 + $.25 per page

The techniques used are based on the methods described in [1] and [2]. In [3], it was pointed out that the method in [2] would fail on a certain class of matrices, and a method was given extending the collection of solvable problems to cover this class. The class in question can be described in terms of the interlacing property

$$\lambda_i \leqslant \mu_i \leqslant \lambda_{i+1}, \qquad i = 1, \ldots, n-1. \tag{2}$$

If the inequalities are strict, then we say J satisfies the *strict interlacing property*. This last property is necessary for the algorithm in [2] but not for the one in [3]. In addition, unlike [2], the method in [3] does not require that the order of the system, n, be even. However the method in [3] starts with substantially different initial data and hence does not directly solve the problem posed in [2].

In this method, we need to assume only that the μ_i be simple. This is equivalent to assuming that the off-diagonal elements of $\bar{J}$ be nonzero [8, p. 300]. In order to ensure that a solution exists in the real numbers, we also need to assume that the λ_i satisfy (2), and that β lies in an interval $(0, \beta_{\max})$, which will be defined below.

2. Preliminaries. We need to define the following two bordered diagonal matrices A, A^- [4] which appear as intermediate results in the course of the computation, and which are similar to J and J^-, respectively, by the same transformation:

$$A = \begin{bmatrix} 1 & 0 \\ 0 & P^T \end{bmatrix} J \begin{bmatrix} 1 & 0 \\ 0 & P \end{bmatrix}, \qquad A^- = \begin{bmatrix} 1 & 0 \\ 0 & P^T \end{bmatrix} J^- \begin{bmatrix} 1 & 0 \\ 0 & P \end{bmatrix}, \tag{3a}$$

where P is the orthogonal matrix of eigenvalues of the submatrix $\bar{J}$. Hence A and J have the same characteristic polynomial, and so do A^- and J^-.

The matrices A, A^-, can be written in the form:

$$A = \begin{bmatrix} a_{11} & \mathbf{c}^T \\ \mathbf{c} & M \end{bmatrix}, \qquad A^- = \begin{bmatrix} a_{11} & (\mathbf{c}^-)^T \\ \mathbf{c}^- & M \end{bmatrix}, \tag{3b}$$

where $M = \operatorname{diag}(\mu_1, \ldots, \mu_{n-1}) = P^T \bar{J} P$, and the eigenvalues of A and A^- are λ_i and λ_i^-, respectively. We shall later see how to define A^- using only β instead of the λ_i^-.

In the following, we will denote the ith row of P as $\mathbf{p}_i^T$, that is $P^T = [\mathbf{p}_1, \ldots, \mathbf{p}_{n-1}]$.

It is obvious that

$$a_{11} = \operatorname{trace}(A) - \operatorname{trace}(M) = \sum_1^n \lambda_i - \sum_1^{n-1} \mu_i. \tag{4a}$$

By expanding the determinant, the characteristic polynomial of A may be written as

$$\det(\lambda I - A) = (\lambda - a_{11}) \prod_{j=1}^{n-1} (\lambda - \mu_j) - \sum_{k=1}^{n-1} c_k^2 \left(\prod_{\substack{j=1, \\ j \neq k}}^{n-1} (\lambda - \mu_j) \right). \tag{4b}$$

Setting $\lambda = \mu_1, \ldots, \mu_{n-1}$ and solving the $n-1$ equations for the c_i yields

$$c_i^2 = -\frac{\prod_{j=1}^{n} (\mu_i - \lambda_j)}{\prod_{j=1; j \neq i}^{n-1} (\mu_i - \mu_j)} \geqslant 0, \tag{4c}$$

thus completely defining A up to the choice of signs of the c_i.

If we let

$$\mathfrak{T} = \begin{bmatrix} a_1 & b_1 & & & & 0 \\ b_1 & a_2 & \cdot & & & \\ & \cdot & \cdot & \cdot & 0 & \\ & & \cdot & \cdot & \cdot & \\ & 0 & & \cdot & a_{n-1} & b_{n-1} \\ 0 & & & & b_{n-1} & a_n \end{bmatrix}$$

and define $p(\lambda)$, $r(\lambda)$ as the charactistic polynomials of the tridiagonal matrices $\mathfrak{T}$ and $\bar{J}$, respectively, then we may write

$$\det(J - \lambda I) = p(\lambda) - b_n^2 r(\lambda) - 2(-1)^n \beta,$$
$$\det(J^- - \lambda I) = p(\lambda) - b_n^2 r(\lambda) + 2(-1)^n \beta.$$

Subtracting yields

$$\det(J^- - \lambda I) = \det(A^- - \lambda I) = \det(A - \lambda I) + 4(-1)^n \beta.$$

So we can solve for c_i^- as in (4c) to obtain

$$(c_i^-)^2 = -\frac{\prod_{j=1}^{n}(\mu_i - \lambda_j) + 4(-1)^n \beta}{\prod_{j=1; j\neq i}^{n-1}(\mu_i - \mu_j)}. \tag{4d}$$

Hence we can define A^-, either with β using (4d), or else by using (4c) with λ_i^- substituted for λ_i. Note that (4d) defines the interval $(0, \beta_{\max})$ in which β must lie by the requirement that $(c_i^-)^2 \geqslant 0$.

If we equate the first columns from Eq. (3a), we get

$$[b_1, 0, \ldots, 0, b_n]^T = P\mathbf{c}, \qquad [b_1, 0, \ldots, 0, -b_n]^T = P\mathbf{c}^-, \tag{5a}$$

in which the left-hand sides are $(n-1)$-vectors. Subtracting yields

$$[0, \ldots, 0, 2b_n]^T = 2b_n \mathbf{e}_{n-1} = P(\mathbf{c} - \mathbf{c}^-),$$

which, applying P^T to both sides, yields

$$2b_n \mathbf{p}_{n-1} = \mathbf{c} - \mathbf{c}^-. \tag{5b}$$

Similarly, if we add the two parts of (5a) together, we get

$$2b_1 \mathbf{p}_1 = \mathbf{c} + \mathbf{c}^-. \tag{5c}$$

In (5b), (5c) the left-hand sides are determined up to sign by the requirement that $\|\mathbf{p}_1\| = \|\mathbf{p}_{n-1}\| = 1$. Note that we have a choice of signs in taking the square roots of the quantities defined in (4c), (4d), to obtain the c_i, c_i^-. A different choice of signs will give rise to different vectors $\mathbf{p}_1, \mathbf{p}_{n-1}$ and hence a different $\bar{J}$. Thus, except in certain degenerate cases, there will be more than one matrix satisfying the initial eigenvalue conditions.

3. The Method. What have we now? We have $\mathbf{p}_1$, that is, the first row of the eigenvector matrix P for a tridiagonal matrix $\bar{J}$. We also have the eigenvalues μ_i of $\bar{J}$, so $\bar{J}$ is completely determined (elementary consequence of Theorem 4.2 of Chapter 7

of [6]). We can compute $\bar{J}$ an element at a time, and P a row at a time, by alternating between the formulas

$$\bar{J} = PMP^T, \tag{6a}$$

$$P^T\bar{J} = MP^T. \tag{6b}$$

The method that results from this is the Lanczos Algorithm [7], [8], and proceeds as follows:

Lanczos Algorithm

Start with $\mathbf{p}_1$ an $(n-1)$-vector with 2-norm 1, and $M = \operatorname{diag}(\mu_1, \ldots, \mu_{n-1})$, a diagonal matrix.

Object: compute orthonormal vectors $\mathbf{p}_2, \ldots, \mathbf{p}_{n-1}$ and an $n-1 \times n-1$ tridiagonal matrix

$$\bar{J} = \begin{bmatrix} t_1 & s_1 & & & & \\ s_1 & t_2 & \cdot & & & 0 \\ & \cdot & \cdot & \cdot & & \\ & & \cdot & \cdot & \cdot & \\ & & & \cdot & \cdot & \cdot \\ & 0 & & & t_{n-2} & s_{n-2} \\ & & & & s_{n-2} & t_{n-1} \end{bmatrix}$$

satisfying (6).

```
1.  begin
2.  t_1 ← p_1^T M p_1;
3.  for i ← 2,..., n − 1 do
4.      begin
5.      z_i ← (if i = 2
                then M p_1 − p_1 t_1
                else M p_{i−1} − p_{i−1} t_{i−1} − p_{i−2} s_{i−2});
6.      s_{i−1} ← ||z_i||_2;
7.      p_i ← z_i / s_{i−1};
8.      t_i ← p_i^T M p_i;
9.      end
10. end.
```

Step 5 is mathematically equivalent to saying

$\mathbf{z}_i \leftarrow M\mathbf{p}_{i-1}$

Orthogonalize $\mathbf{z}_i$ against all $\mathbf{p}_{i-1}, \ldots, \mathbf{p}_1$ by Gram-Schmidt.

What was actually implemented was the original step 5, followed by a complete Gram-Schmidt reorthogonalization. The Lanczos Algorithm is stable only if some reorthogonalization is used [11, Theorems 2.3, 2.4, 2.5], and for simplicity we chose to use complete reorthogonalization.

In step 7, $s_{i-1} \neq 0$ is guaranteed from the assumption that the eigenvalues μ_i are distinct [8, p. 300].

It must be noted that the tridiagonal matrix $\bar{J}$ may be constructed by using Householder Transformations instead of using the Lanczos Algorithm with complete reorthogonalization. The details are given in [4], and this method can be substituted

for the Lanczos algorithm giving theoretically equivalent results. However, it was noted in [4] that the method using Householder Transformations is more expensive, but on badly conditioned problems it may be more stable, depending on the kind of reorthogonalization used [11]. On the other hand, the Lanczos Algorithm is much more suited for large sparse problems. Further comparison between the methods is necessary.

The algorithm to reconstruct J is then as follows:

Reconstruction Algorithm

Compute the $n-1 \times n-1$ submatrix $\bar{J}$ (defined just below (1a)):

1. Compute $\mathbf{c}, \mathbf{c}^-$ using (4c), (4d).
2. Compute b_i and $\mathbf{p}_1$ by (5c) subject to $\|\mathbf{p}_1\|_2 = 1$.
3. Apply the Lanczos Algorithm starting with vector $\mathbf{p}_1$ and matrix $M = \operatorname{diag}(\mu_1, \ldots, \mu_{n-1})$, obtaining vectors P and tridiagonal matrix $\bar{J}$.

Fill in the first row and column of J defined in (1a):

4. Compute $a_1 = \Sigma_1^n \lambda_i - \Sigma_1^{n-1} \mu_i$ (Eq. (4a)).
5. Compute b_n by either (5b) or from the definition of β:

$$b_n = \frac{\beta}{(b_1 \cdots b_{n-1})}.$$

4. Numerical Results. A RATFOR program has been written to test this method. It successfully reconstructed the example suggested in [3], with $n = 4, 5, 6$, namely

$$J = \begin{bmatrix} 2 & 1 & & & & & 1 \\ 1 & 2 & \cdot & & & & \\ & \cdot & \cdot & \cdot & & 0 & \\ & & \cdot & \cdot & \cdot & & \\ & 0 & & \cdot & \cdot & \cdot & \\ & & & & \cdot & 2 & 1 \\ 1 & & & & & 1 & 2 \end{bmatrix},$$

for which the μ_i are simple, but the λ_i are not. The initial data used in these test cases, as well as the vectors $\mathbf{c}, \mathbf{c}^-$, are listed below:

$n = 4, \beta = 1$

initial λ_i	initial μ_i	c_i	c_i^-
0	0.58578644	1.00000000	0
2.00000000	2.00000000	0	1.41421356
2.00000000	3.41421356	1.00000000	0
4.00000000	–	–	–

$n = 5, \beta = 1$

initial λ_i	initial μ_i	c_i	c_i^-
0.38196601	0.38196601	0	0.74349607
0.38196601	1.38196601	1.20300191	0
2.61803399	2.61803399	0	1.20300191
2.61803399	3.61803399	0.74349607	0
4.00000000	–	–	–

$n = 6, \beta = 1$

initial λ_i	initial μ_i	c_i	c_i^-
0	0.26794919	0.57735027	0
1.00000000	1.00000000	0	1.00000000
1.00000000	2.00000000	1.15470054	0
3.00000000	3.00000000	0	1.00000000
3.00000000	3.73205081	0.57735027	0
4.00000000	–	–	–

The following example illustrates the fact that the b_i need not be positive. This example is simply the J^-, defined by (1b), corresponding to the J used in the above case $n = 4$.

$n = 4, \beta = -1$

initial λ_i	initial μ_i	c_i	c_i^-
0.58578644	0.58578644	0	1.00000000
0.58578644	2.00000000	1.41421356	0
3.41421356	3.41421356	0	1.00000000
3.41421356	–	–	–

The above cases all have remarkable property that for all i, $i = 1, \ldots, n-1$, either $c_i = 0$ or $c_i^- = 0$, so that the reconstructed matrix J is essentially unique (up to signs of the off-diagonal elements). In the following example, we show a more general case, in which the answer is not unique. The results were obtained by starting with one set of eigenvalue data and cycling through all possible sign combinations for the c_i, c_i^-. The initial data and the **c** vectors were:

$n = 4, \beta = .25$

initial λ_i	initial μ_i	c_i	c_i^-
0	0.58578644	1.00000000	0.86602540
2.00000000	2.00000000	0	0.70710678
2.00000000	3.41421356	1.00000000	0.86602540
4.00000000	–	–	–

The 4 distinct matrices that were computed are given below. For brevity, we show each distinct matrix only once, since each one actually appeared 8 times. Since there were no degeneracies encountered in this example, and by observing that any matrix satisfying the initial conditions (given by λ_i, μ_i, β) must satisfy (4a)–(4d) and (5c), it follows that the following are all the possible distinct answers for the given initial data above.

a_i	b_i
2.00000000	1.36602540
2.00000000	1.36602540
2.00000000	0.36602540
2.00000000	0.36602540

a_i	b_i
2.00000000	0.36602540
2.00000000	0.36602540
2.00000000	1.36602540
2.00000000	1.36602540
a_i	b_i
2.00000000	1.00000000
0.77525513	0.50000000
2.00000000	0.50000000
3.22474487	1.00000000
a_i	b_i
2.00000000	1.00000000
3.22474487	0.50000000
2.00000000	0.50000000
0.77525513	1.00000000

As a final example, we tried the example 3 of Table 2 on page 1218 of [3], in which the matrices in question were reconstructed only with large errors. The matrices are defined as follows, for $n = 5, 10, 15, 20, 25, 30$:

$$a_i = \frac{i}{n} - 2, \qquad i = 1, \ldots, n-1,$$

$$b_i = 1 - \frac{i}{n}, \qquad i = 1, \ldots, n-2,$$

$$b_n = b_{n-1} = 1,$$

$$a_n = 0.$$

The algorithm was suitably modified to account for the fact that the submatrix $\bar{J}$ in this example was obtained by deleting the last row and column rather than the first.

Unfortunately, there are too many combinations of signs for the c_i, c_i^- to compute all the possible matrices. For $n = 10$ alone there are 262144 different choices of signs. However, in each case we are able to compare the eigenvalues of the reconstructed matrix with the initial eigenvalues. Since the eigenvalues for symmetric matrices are always well-conditioned, the discrepancy between the two sets of eigenvalues is a good indicator of the error in the reconstructed matrices.

n	Norm of discrepancy
5	.364539663e − 15
10	.558570184e − 15
15	.130290552e − 14
20	.191718261e − 14
25	.304003744e − 14
30	.340721065e − 14

Here, the norm of discrepancy is the square root of the sum of the squares of the differences between the two sets of eigenvalues.

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