

for $j = 1, 2, \dots, N - 1$. But this is impossible, for no matrix of order $l < N - 1$ has $N - 1$ distinct eigenvalues.

Second, we will demonstrate that the numbers $Y_{i,j}$, computed by this algorithm, form the entries of an orthogonal matrix Y . That is, the rows of Y satisfy the orthonormality relations

$$(6) \quad \sum_{k=1}^{N-1} Y_{i,k} Y_{j,k} = \delta_{i,j} \quad \text{for } j = 1, 2, \dots, i,$$

and $i = 1, 2, \dots, N - 1$. From the compatibility of the data we infer that (6) is true for $i = 1$. If (6) is true for $i = 1, 2, \dots, l$, then the following argument demonstrates that it is also true for $i = l + 1$. Clearly steps 6 and 7 imply that (6) is true for $j = l + 1$. For $j \leq l$ step 7 implies that

$$\sum_{k=1}^{N-1} Y_{l+1,k} Y_{j,k} = \frac{1}{b_l} \left[\sum_{k=1}^{N-1} \mu_k Y_{l,k} Y_{j,k} - a_l \delta_{l,j} - b_{l-1} \delta_{l-1,j} \right].$$

Since step 5 was executed, the right side of this equality is zero for $j = l$. The right side of this equality is also zero for $j < l$ because step 7 implies that

$$\sum_{k=1}^N \mu_k Y_{l,k} Y_{j,k} = \sum_{k=1}^{N-1} Y_{l,k} [b_{j-1} Y_{j-1,k} + a_j Y_{j,k} + b_j Y_{j+1,k}] = b_j \delta_{l,j+1}.$$

Third, we will demonstrate that the data $\{\mu, y\}$ characterizes J . It will be sufficient to prove that the matrices J, Y constructed by this algorithm satisfy (1). Step 7 implies that $JY = YD$ if we can show that the numbers

$$Y_{N,j} \equiv (\mu_j - a_j) Y_{N-1,j} - b_{N-2} Y_{N-2,j}$$

are zero for $j = 1, 2, \dots, N - 1$. The techniques presented in the previous paragraph can be used to demonstrate that

$$\sum_{k=1}^{N-1} Y_{N,k} Y_{j,k} = 0 \quad \text{for } j = 1, 2, \dots, N - 1.$$

Since the rows of Y form a real, orthonormal basis for \mathbf{R}^{N-1} , we infer that

$$Y_{N,j} = 0 \quad \text{for } j = 1, 2, \dots, N - 1. \quad \square$$

LEMMA 2.5. *Each set of compatible data characterizes at most one Jacobi matrix.*

Proof. Let \hat{J} be any Jacobi matrix characterized by the compatible data $\{\mu, y\}$. Then y_1, y_2, \dots, y_{N-1} are the first components of a set $\hat{Y}_1, \hat{Y}_2, \dots, \hat{Y}_{N-1}$ of real, orthonormal eigenvectors of \hat{J} corresponding to the eigenvalues $\mu_1, \mu_2, \dots, \mu_{N-1}$. If \hat{Y} denotes the matrix whose j th column is \hat{Y}_j , then \hat{Y} is an orthogonal matrix and

When both sides are integrated with respect to ρ , we find that

$$\det(\lambda I - L_\rho) = b_1 b_2 \cdots b_N \left\{ \Delta(\lambda) - \left(\rho + \frac{1}{\rho} \right) \right\}.$$

Of course, the constant of integration $b_1 b_2 \cdots b_N \Delta(\lambda)$ is necessarily independent of ρ .

Let J be characterized by the data $\{\mu, y\}$. Then y_1, y_2, \dots, y_{N-1} are the first components of a set Y_1, Y_2, \dots, Y_{N-1} of real, orthonormal eigenvectors of J corresponding to its eigenvalues $\mu_1, \mu_2, \dots, \mu_{N-1}$. Let $Y_{i,j}$ denote the i th component of Y_j . From the definition (7) of the Floquet multipliers and the identity (5), we infer that

$$\rho_j = -\frac{b_{N-1} Y_{N-1,j}}{b_N Y_{1,j}} \quad \text{for } j = 1, 2, \dots, N-1,$$

and so

$$L_{\rho_j} \begin{bmatrix} Y_j \\ 0 \end{bmatrix} = \mu_j \begin{bmatrix} Y_j \\ 0 \end{bmatrix} \quad \text{for } j = 1, 2, \dots, N-1.$$

Consequently μ_j is an eigenvalue of L_{ρ_j} for $j = 1, 2, \dots, N-1$, and we infer from (8) that (9) is true.

From the definition (7) of the Floquet multipliers, we deduce that

$$\omega'_j(\mu_j) \rho_j < 0 \quad \text{for } j = 1, 2, \dots, N-1.$$

When the eigenvalues $\mu_1, \mu_2, \dots, \mu_{N-1}$ of J are ordered so that $\mu_1 > \mu_2 > \dots > \mu_{N-1}$, we infer from (9) that

$$(-1)^j \Delta(\mu_j) \geq 2 \quad \text{for } j = 1, 2, \dots, N-1,$$

because the magnitude of $\rho + 1/\rho$ is never less than two. Consequently the eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_N$ of L , which are the roots of $\Delta = 2$, are real and can be ordered so that $\lambda_1 > \lambda_2 \geq \lambda_3 > \lambda_4 \geq \lambda_5 > \dots$, because the coefficient $(b_1 b_2 \cdots b_N)^{-1}$ of λ^N in Δ is positive. \square

A typical discriminant of a Jacobi matrix L of order $N = 6$ is illustrated in Figure 1. In this figure we have depicted the relationship between the eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_N$ of L and the Floquet multipliers $\rho_1, \rho_2, \dots, \rho_{N-1}$ of L corresponding to the eigenvalues $\mu_1, \mu_2, \dots, \mu_{N-1}$ of J .

Definition 3.3. (a) The periodic Jacobi matrix L is characterized by the data $\{A, B, \mu, \rho\}$ if and only if

- (1) $A = a_1 + a_2 + \dots + a_N$,
- (2) $B = b_1 b_2 \cdots b_N$,
- (3) $\mu_1, \mu_2, \dots, \mu_{N-1}$ are the eigenvalues of J , and
- (4) $\rho_1, \rho_2, \dots, \rho_{N-1}$ are the Floquet multipliers of L corresponding to $\mu_1, \mu_2, \dots, \mu_{N-1}$.

(b) The data $\{A, B, \mu, \rho\}$ are compatible if and only if

- (1) A is a real number,
- (2) B is a real, positive number,
- (3) $\mu_1, \mu_2, \dots, \mu_{N-1}$ are real, distinct numbers, and
- (4) $\rho_1, \rho_2, \dots, \rho_{N-1}$ are real numbers which satisfy $\omega'(\mu_j)\rho_j < 0$ for $j = 1, 2, \dots, N-1$ with $\omega(\mu) = (\mu - \mu_1)(\mu - \mu_2) \cdots (\mu - \mu_{N-1})$.

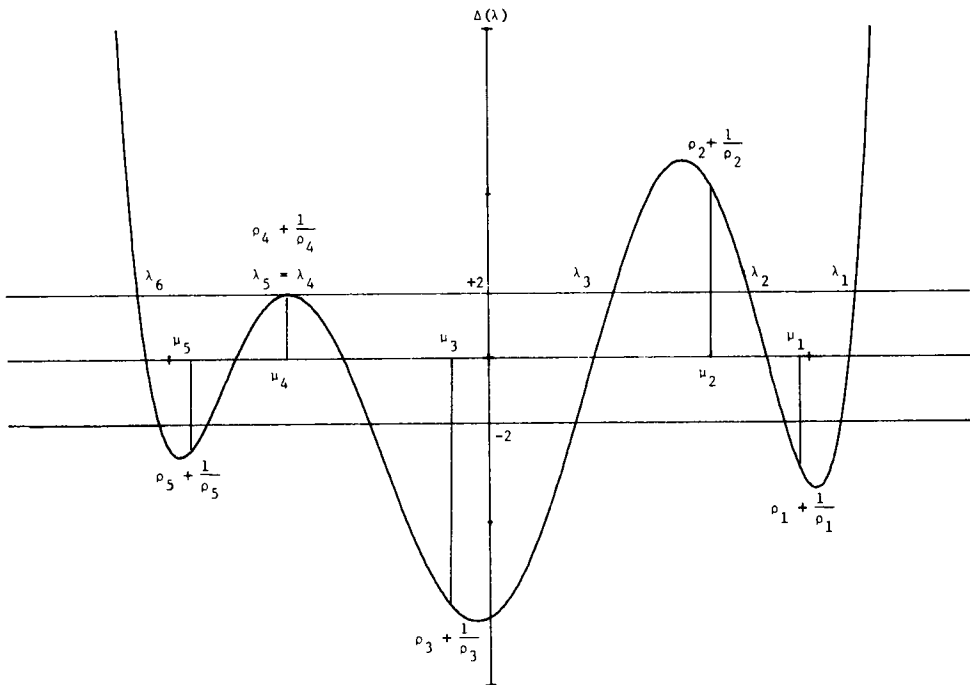


FIGURE 1

Plot of a typical discriminant, $N = 6$

We feel justified in using the words “characterize” and “compatible” in this manner because the following theorem is true.

THEOREM 3.4. *Data characterizing a periodic Jacobi matrix are compatible. Furthermore, each set of compatible data $\{A, B, \mu, \rho\}$ characterizes a unique periodic Jacobi matrix L . The entries (a, b) of this periodic Jacobi matrix L are computed by the algorithm:*

1. $b_N = +\sqrt{-\sum_{k=1}^{N-1} (B/\rho_k \omega'(\mu_k))}$;
2. $y_j = (1/b_N) + \sqrt{-(B/\rho_j \omega'(\mu_j))}$ for $j = 1, 2, \dots, N-1$;
3. Recover the Jacobi matrix J characterized by the data $\{\mu, y\}$;
4. $b_{N-1} = B/b_1 b_2 \cdots b_{N-2} b_N$;
5. $a_N = A - (a_1 + a_2 + \cdots + a_{N-1})$;

where $\omega(\mu) = (\mu - \mu_1)(\mu - \mu_2) \cdots (\mu - \mu_{N-1})$.

Proof. The proof of this theorem will be presented as a sequence of three lemmas. \square

LEMMA 3.5. *Data characterizing a periodic Jacobi matrix are compatible.*

Proof. Let the data $\{A, B, \mu, \rho\}$ characterize the periodic Jacobi matrix L . Clearly A is a real number and B is a real, positive number. The μ_j 's are real, distinct numbers since they are the eigenvalues of the Jacobi matrix J . The definition (7) of the ρ_j 's makes it obvious that they are real, nonzero numbers which satisfy $\omega'(\mu_j)\rho_j < 0$ for $j = 1, 2, \dots, N - 1$ because ω is also the characteristic polynomial of J . \square

LEMMA 3.6. *Given compatible data $\{A, B, \mu, \rho\}$, the algorithm of Theorem 3.4 computes the entries (a, b) of a periodic Jacobi matrix L characterized by the data $\{A, B, \mu, \rho\}$.*

Proof. The data $\{\mu, \gamma\}$ used in step 3 in the algorithm of Theorem 3.4 are compatible, therefore it is clear that this algorithm computes the entries (a, b) of some periodic Jacobi matrix L . Let L be characterized by the data $\{\hat{A}, \hat{B}, \hat{\mu}, \hat{\rho}\}$. From steps 4 and 5 of this algorithm it is clear that $\hat{A} = A$ and $\hat{B} = B$. In view of Theorem 2.2 we know that J is characterized by the data $\{\mu, \gamma\}$. Therefore $\hat{\mu}_j = \mu_j$ for $j = 1, 2, \dots, N - 1$, and from the definition of the Floquet multipliers we know that

$$B = -\hat{\rho}_j \omega'(\mu_j) b_N^2 \gamma_j^2 \quad \text{for } j = 1, 2, \dots, N - 1.$$

Step 2 of this algorithm therefore implies that $\hat{\rho}_j = \rho_j$ for $j = 1, 2, \dots, N - 1$. \square

LEMMA 3.7. *Each set of compatible data characterizes at most one periodic Jacobi matrix.*

Proof. Let \hat{L} be any periodic Jacobi matrix characterized by the data $\{A, B, \mu, \rho\}$. Let the Jacobi matrix \hat{J} , obtained from \hat{L} by deleting the last row and column, be characterized by the data $\{\mu, \hat{\gamma}\}$. As pointed out at the end of Section 2, we may assume that each $\hat{\gamma}_j$ is positive. We will now prove that the entries (\hat{a}, \hat{b}) of \hat{L} are identical to the entries (a, b) of the periodic Jacobi matrix L constructed by the algorithm of Theorem 3.4.

By definition the Floquet multipliers $\rho_1, \rho_2, \dots, \rho_{N-1}$ of \hat{L} corresponding to $\mu_1, \mu_2, \dots, \mu_{N-1}$, satisfy the relationship

$$B = -\rho_j \omega'(\mu_j) \hat{b}_N^2 \hat{\gamma}_j^2 \quad \text{for } j = 1, 2, \dots, N - 1.$$

The sum of the squares of the $\hat{\gamma}_j$'s equals one because the data $\{\mu, \hat{\gamma}\}$ is compatible, therefore

$$\hat{b}_N^2 = - \sum_{k=1}^{N-1} \frac{B}{\rho_k \omega'(\mu_k)},$$

and

$$\hat{\gamma}_j^2 = - \frac{B}{b_N^2 \rho_j \omega'(\mu_j)} \quad \text{for } j = 1, 2, \dots, N - 1.$$

In view of steps 1 and 2 of this algorithm, we infer that $\hat{b}_N = b_N$ and $\hat{\gamma}_j = \gamma_j$ for $j = 1, 2, \dots, N - 1$. Since J and \hat{J} are characterized by the same data, Theorem 2.2 implies that $J = \hat{J}$. Finally, steps 4 and 5 of this algorithm imply that $\hat{b}_{N-1} = b_{N-1}$ and $\hat{a}_N = a_N$. \square

Proof. If the data $\{A, B, \mu, \rho\}$ characterizes a member of $F(p)$, then Theorems 3.2 and 3.4 demonstrate that conditions (1), (2), (3) are satisfied. Now suppose the data $\{A, B, \mu, \rho\}$ satisfies (1), (2), (3). Let Δ be the discriminant of the periodic Jacobi matrix characterized by $\{A, B, \mu, \rho\}$. Now

$$q = \Delta - p$$

is a polynomial of degree $N - 2$ because the coefficients of λ^N, λ^{N-1} in $\Delta(\lambda), p(\lambda)$ are identical. Theorem 3.2 implies that

$$q(\mu_j) = 0 \quad \text{for } j = 1, 2, \dots, N - 1,$$

and so $q \equiv 0$ because the only polynomial of degree $N - 2$ which is zero at $N - 1$ distinct points is the trivial polynomial. Therefore, the data $\{A, B, \mu, \rho\}$ characterizes a member of $F(p)$.

If $F(p)$ is nonempty, then conditions (2), (3) and the mean-value theorem can be used to demonstrate that conditions (4), (5) are satisfied. Let us now suppose that p satisfies conditions (4), (5). Determine A, B so that

$$p(\lambda) = \frac{1}{B} [\lambda^N - A\lambda^{N-1} + \text{lower powers of } \lambda],$$

and define $\rho_1, \rho_2, \dots, \rho_{N-1}$ to be solutions of

$$p(v_j) = \rho_j + \frac{1}{\rho_j} \quad \text{for } j = 1, 2, \dots, N - 1.$$

Then the data $\{A, B, \mu, \rho\}$ are compatible and from (1), (2), (3) we infer that the data $\{A, B, \mu, \rho\}$ characterizes a member of $F(p)$. \square

Using Theorem 4.2, we can now characterize the family of Jacobi matrices having $\lambda_1, \lambda_2, \dots, \lambda_N$ as its eigenvalues.

THEOREM 4.3. *The periodic Jacobi matrix L has $\lambda_1, \lambda_2, \dots, \lambda_N$ as its eigenvalues if and only if*

$$L \in \bigcup_{B>0} F(\Delta_B),$$

where

$$\Delta_B(\lambda) = 2 + \frac{1}{B} (\lambda - \lambda_1)(\lambda - \lambda_2) \cdots (\lambda - \lambda_N).$$

Furthermore, there is a family of periodic Jacobi matrices with $\lambda_1, \lambda_2, \dots, \lambda_N$ as its eigenvalues if and only if the numbers can be rearranged so that $\lambda_1 > \lambda_2 \geq \lambda_3 > \lambda_4 \geq \lambda_5 > \dots$.

Parts of Theorems 4.2 and 4.3 appear in the work of van Moerbeke [15]. For example, in Theorem 2.1 of [15] van Moerbeke parametrizes the family of periodic Jacobi matrices having $\lambda_1, \lambda_2, \dots, \lambda_N$ as their eigenvalues provided there is at least one periodic Jacobi matrix with these eigenvalues.

5. Numerical Experiments. We will now present the results of several numerical experiments. These experiments were carried out on a UNIVAC 1110 in single-precision floating-point binary arithmetic (27 bit mantissa) using FORTRAN versions of the algorithms presented in Theorems 2.2 and 3.4.

In the first experiment we tested the algorithm presented in Theorem 2.2. The results of this experiment are presented in Table 1. Observe that this algorithm has difficulty in recovering the Jacobi matrix described in Example 3.

Experiment 1. Test the algorithm for Jacobi matrices.

1. Select a Jacobi matrix J of order $N - 1$.
2. Compute the data $\{\mu, \gamma\}$ characterizing J [17], [18]:
 - (a) use bisection to compute the μ_j 's and
 - (b) use inverse iteration to compute the γ_j 's.
3. Use the algorithm presented in Theorem 2.2 to reconstruct the Jacobi matrix \hat{J} characterized by the data $\{\mu, \gamma\}$.
4. Output the error $\|J - \hat{J}\|$, where $\|A\| = \max_{i,j} |a_{i,j}|$.

In the second experiment we tested the algorithm presented in Theorem 3.4. The results of this experiment are presented in Table 2. Observe that the Jacobi matrices used in the examples of Experiment 1 are obtained by deleting the last row and column from the periodic Jacobi matrices used in the corresponding examples of Experiment 2.

Experiment 2. Test the algorithm for periodic Jacobi matrices.

1. Select a periodic Jacobi matrix L of order N .
2. Compute the data $\{A, B, \mu, \rho\}$ characterizing L :
 - (a) $A = a_1 + a_2 + \cdots + a_N$,
 - (b) $B = b_1 b_2 \cdots b_N$,
 - (c) compute the data $\{\mu, \gamma\}$ characterizing J as described in step 2 of Experiment 1,
 - (d) compute the ρ_j 's using (7).
3. Use the algorithm presented in Theorem 3.4 to reconstruct the periodic Jacobi matrix L characterized by the data $\{A, B, \mu, \rho\}$.
4. Output the error $\|L - \hat{L}\|$, where $\|A\| = \max_{i,j} |a_{i,j}|$.

TABLE 1. *Results of Experiment 1*

Example 1:

$A(I) = -2$	$I = 1, \dots, N - 1$
$B(I) = 1$	$I = 1, \dots, N - 2$
N	Error
5	4×10^{-8}
10	2×10^{-7}
15	5×10^{-7}
20	2×10^{-7}
25	2×10^{-7}
30	6×10^{-7}

Example 2:

$A(I) = (N + 1 - I)/N - 2$	$I = 1, \dots, N - 1$
$B(I) = 1 - (N - I)/N$	$I = 1, \dots, N - 2$
N	Error
5	4×10^{-8}
10	1×10^{-7}
15	4×10^{-7}
20	3×10^{-7}
25	3×10^{-7}
30	9×10^{-7}

Example 3:

$A(I) = I/N - 2$	$I = 1, \dots, N - 1$
$B(I) = 1 - I/N$	$I = 1, \dots, N - 2$
N	Error
5	1×10^{-7}
10	3×10^{-7}
15	2×10^{-4}
20	2×10^0
25	2×10^0
30	1×10^0

TABLE 2. Results of Experiment 2

Example 1:

$A(I) = -2$	$I = 1, \dots, N - 1$
$B(I) = 1$	$I = 1, \dots, N - 2$
$A(N) = 0$	
$B(N - 1) = B(N) = 1$	
N	Error
5	9×10^{-8}
10	5×10^{-7}
15	1×10^{-6}
20	2×10^{-6}
25	3×10^{-6}
30	5×10^{-6}

Example 2:

$$\begin{aligned} A(I) &= (N + 1 - I)/N - 2 & I = 1, \dots, N - 1 \\ B(I) &= 1 - (N - I)/N & I = 1, \dots, N - 2 \\ A(N) &= 0 \\ B(N - 1) &= B(N) = 1 \end{aligned}$$

N	Error
5	1×10^{-7}
10	2×10^{-7}
15	4×10^{-7}
20	3×10^{-7}
25	6×10^{-7}
30	4×10^{-7}

Example 3:

$$\begin{aligned} A(I) &= I/N - 2 & I = 1, \dots, N - 1 \\ B(I) &= 1 - I/N & I = 1, \dots, N - 2 \\ A(N) &= 0 \\ B(N - 1) &= B(N) = 1 \end{aligned}$$

N	Error
5	4×10^{-8}
10	1×10^{-7}
15	1×10^{-3}
20	2×10^0
25	4×10^0
30	5×10^0

In both of these experiments we have not worked with matrices of order N greater than thirty. In Example 2 of Experiment 2 some of the components of y in the data $\{\mu, y\}$ characterizing J become smaller as N increases. For example, the smallest component of y changes from $O(10^{-9})$ for $N = 15$ to $O(10^{-20})$ for $N = 30$. Since the Floquet multipliers ρ_j depend on the squares of the corresponding y_j , we would therefore run into underflow problems. The immediate remedy for this underflow problem is to compute the logarithms of each ρ_j instead of ρ_j . However, underflow also occurs in the computation of the y_j 's when N is greater than fifty-five.

6. Comments. It is interesting to note that the Lanczos algorithm of Theorem 2.2 is used in some versions of the implicit shift QR algorithm [16]. These versions of the QR algorithm make use of the fact that if $B = QAQ^H$, where B is an unreduced upper Hessenberg matrix and Q is a unitary matrix, then the entries of B and Q are uniquely determined from the entries of A and the entries in the first row of Q . In our application we have $A = D$, $Q = Y$, and $B = J$!

