On the Calculation of Jacobi Matrices

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Dedicated to A. M. Ostrowski
on the occasion of his ninetieth birthday.

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ABSTRACT

Given a Jacobi matrix, the problem in question is to find the Jacobi matrix corresponding to the weight function modified by a polynomial r. Galant and Gautschi derived algorithms, based on the generalized Christoffel theorem of Uvarov, applicable when the roots of r are known. In this paper we present two methods not requiring the explicit knowledge of the roots of r. We also obtain various properties of the similarity transformations between Jacobi matrices, which we prove by simple matrix calculus without using the generalized Christoffel theorem.

1. INTRODUCTION

Polynomials orthonormal with respect to a nonnegative weight function (for which the monomial moments exist) satisfy a three-term recurrence relation. Coefficients of this relation form a symmetric tridiagonal matrix—called a Jacobi matrix—the eigenvalues of which are the roots of the

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orthogonal polynomial of the degree equal to the order of the Jacobi matrix. The knowledge of the Jacobi matrix thus not only is important for the determination of the orthonormal polynomials, but leads also to stable and efficient methods for solving various problems involving Gaussian and interpolatory quadratures [7–10].

The Jacobi matrix is explicitly known for some particular weight functions (see e.g. Table 2 in [10]). Generally it could be evaluated by an inverse Cholesky decomposition of the matrix of moments (Gram-Schmidt orthogonalization; see Theorem 2 in Section 2), but this process is usually very unstable, due to the condition of the moment matrix. Another approach is to seek, say, the Jacobi matrix $\tilde{J}$ for a given weight function $\tilde{w}$ as a modification of a known Jacobi matrix J for some weight function w. In fact, only the ratio $f := \tilde{w}/w$ determines the modifying process. Two questions immediately arise: (1) for what functions f can we perform such a modification effectively, and (2) how does an approximation of a general $\tilde{w}/w$ by an f of the form for which the modification is possible affect the accuracy of the resulting matrix $\tilde{J}$? In this paper we will be concerned mainly with the first question. Uvarov [12, 13] has formulated the generalized Christoffel theorem which expresses the polynomials orthogonal with respect to $\tilde{w}$ in terms of those orthogonal with respect to w in the case when f is a rational function with known linear factors. Gautschi [6] obtained algorithms for modifying the coefficients of the three term relation for monic orthogonal polynomials (rather than orthonormal polynomials; however, chosing the polynomials monic makes no essential difference to the formulation of the problem). Galant [2] derived a similar algorithm earlier for a polynomial (rather than rational) modification f and has pointed out that each linear factor modification is equivalent to one step of a symmetric LR method with a shift. As a consequence, it should be possible to perform the modification by a square of a linear factor—two steps of a symmetric LR method—as one step of a QR method. We have demonstrated this in [9] and have given simple proofs of the relations between the modified matrix $\tilde{J}$ and the matrix, similar to J, obtained by such transformations. Using similar means—i.e. using global properties of the matrices involved without relying on the generalized Christoffel theorem of Uvarov—we show in this paper that the modification by a polynomial of any degree can be achieved by either a Lanczos type process or, if the diagonalization of J is available, by one step of the implicit QR method. The latter process appears to be superior in numerical stability when the modifying polynomial f has multiple roots close to the support of the weight function.

In Section 2 we study transformations between polynomial bases, arbitrary or orthogonal, which we express using matrices of coefficients of recurrence relations satisfied by the polynomials in question. The main results are presented in Section 3 and formulated as numerical methods in Section 4.

In the last section we report and assess numerical experiments with these methods.

2. TRANSFORMATIONS OF POLYNOMIAL BASES

In this section we establish basic relations between the lower Hessenberg (and, in particular, Jacobi) matrices corresponding to different polynomial bases.

To start, we note that there is a simple correspondence between such matrices and polynomial bases of exact degree. Given integer $k > 1$, $\beta_k \neq 0$, $P_0 \neq 0$, and a proper lower Hessenberg matrix J of order k (i.e. with nonzero superdiagonal elements denoted, say, $\beta_1, \dots, \beta_{k-1}$), there exist polynomials p_j of exact degree j, $j = 0, 1, 2, \dots, k$, such that the identity

$$t\mathbf{p}(t) = J\mathbf{p}(t) + \beta_k p_k(t)\mathbf{e}_k \tag{2.1}$$

holds for all t. Here, and throughout this paper, we denote $\mathbf{p} := (p_0, p_1, \dots, p_{k-1})^T$ and $\mathbf{e}_k$ the kth unit vector of an appropriate dimension. Similarly, given a polynomial basis $\mathbf{p}$, p_k (of exact degree), there is a unique $\beta_k \neq 0$ and a unique proper lower Hessenberg matrix J satisfying (2.1).

In what follows we shall always assume $\beta_j > 0$; as this can be achieved by a change of signs of the basis polynomials, there is no loss of generality. The following lemma is the first step in our investigation of the relations between two polynomial bases.

LEMMA 1. *Given two proper lower Hessenberg matrices J and $\tilde{J}$, there exist a unique (up to a scalar factor) nonsingular lower triangular matrix L and vector $\mathbf{c}$ such that*

$$L\tilde{J} = JL + \mathbf{e}_k\mathbf{c}^T. \tag{2.2}$$

Furthermore, given $\beta_k \neq 0 \neq \tilde{\beta}_k$, if $\mathbf{p}$, p_k and $\tilde{\mathbf{p}}$, $\tilde{p}_k$ are the polynomial bases corresponding to J, β_k and $\tilde{J}$, $\tilde{\beta}_k$, respectively, then

$$\mathbf{p} = L\tilde{\mathbf{p}}, \tag{2.3a}$$

$$\beta_k p_k - \tilde{\beta}_k \tilde{p}_k \mathbf{e}_k^T L \mathbf{e}_k = \mathbf{c}^T \tilde{\mathbf{p}}. \tag{2.3b}$$

Proof. As $\mathbf{p}$ and $\tilde{\mathbf{p}}$ are polynomial bases of exact degree, there exists a nonsingular lower triangular matrix L satisfying (2.3a). This matrix is unique up to a factor depending on the ratio $p_0/\tilde{p}_0$, which we can choose arbitrarily when choosing the polynomial bases. Substituting (2.3a) into (2.1) and subtracting a similar identity for $\tilde{J}, \tilde{\beta}_k, \tilde{\mathbf{p}}, \tilde{p}_k$ (premultiplied by L), we obtain

$$(JL - L\tilde{J})\tilde{\mathbf{p}} + \left(\beta_k p_k - \tilde{\beta}_k \tilde{p}_k \mathbf{e}_k^T L \mathbf{e}_k\right)\mathbf{e}_k = \mathbf{0}.$$

The scalar in the second term must be a polynomial of degree less than k (as is the first term), say $\mathbf{c}^T\tilde{\mathbf{p}}$ for some vector $\mathbf{c}$. The equation (2.2) then follows by substitution from the above identity. ■

We are now interested in a reversed problem. Given J and $\mathbf{c}$, but not knowing L, is the matrix $\tilde{J}$ determined by the equation (2.2)? The situation is similar to that which leads to the Lanczos method except that the orthogonal transformation matrix is replaced by a lower triangular one. Algorithm 1 below gives an explicit construction of the matrix $\tilde{J}$ satisfying (2.2) assuming, as in the Lanczos method, that $\tilde{J}$ is symmetric (and therefore tridiagonal) and that the first column $\mathbf{u} := L\mathbf{e}_1$ of the transformation matrix is known with $\mathbf{e}_1^T\mathbf{u} > 0$.

ALGORITHM 1. *Input*: Matrix J (order k), vectors $\mathbf{u}, \mathbf{c}$ (dimension k).

Step 1: *Set* $\mathbf{v}_0 := \mathbf{0}$, $\mathbf{v}_1 := \mathbf{u}$, $\gamma_1 := 1$, $\tilde{\beta}_0 := 1$, $\lambda_1 := (\mathbf{e}_1^T\mathbf{v}_1)^{-1}$, $\tilde{\alpha}_1 := \lambda_1 \mathbf{e}_1^T J \mathbf{v}_1$.

Step 2: *For* $j = 2, 3, \ldots, k$ *do*

set $\mathbf{v}_j := ((J - \tilde{\alpha}_{j-1} I)\mathbf{v}_{j-1} - \gamma_{j-1}\mathbf{v}_{j-2})/\tilde{\beta}_{j-2} + \mathbf{c}^T \mathbf{e}_{j-1}\mathbf{e}_k$,

$\gamma_j := \lambda_{j-1}\mathbf{e}_{j-1}^T J \mathbf{v}_j$,

$\lambda_j := (\mathbf{e}_j^T\mathbf{v}_j)^{-1}$,

$\tilde{\beta}_{j-1} := (\gamma_j \tilde{\beta}_{j-2})^{1/2}$,

$\tilde{\alpha}_j := \lambda_j \mathbf{e}_j^T (J\mathbf{v}_j - \gamma_j \mathbf{v}_{j-1} + \tilde{\beta}_{j-1}\mathbf{e}_j^T \mathbf{c}\, \mathbf{e}_k)$.

Output: Matrix $\tilde{J} = \begin{pmatrix} \tilde{\alpha}_1 & \tilde{\beta}_1 & 0 & \cdots & 0 \\ \tilde{\beta}_1 & \tilde{\alpha}_2 & \tilde{\beta}_2 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & \tilde{\alpha}_k \end{pmatrix}$

For brevity we have omitted to test if $\lambda_j > 0$, which of course might fail, depending on the input $\mathbf{u}$ (we assume $\beta_j := \mathbf{e}_j^T J \mathbf{e}_{j+1} > 0$, for which we then have in Step 2 that $\gamma_j := \lambda_{j-1}\beta_{j-1}/\lambda_j > 0$ so that $\tilde{\beta}_{j-1}^2 > 0$). In Section 5 we shall mention examples where, however, $\tilde{\beta}_{j-1}^2 < 0$ due to roundoff errors.

We are also interested in how the vector $\mathbf{c}$ affects the result. To express this we use the following terminology. The mth perdiagonal of a matrix $A = (a_{ij})_{i,j=1}^n$ is formed by elements a_{ij} such that $i + j = m + 1$. Also, by $\mathbb{Z}_{k,m}$ (or $\mathbb{Z}_m$, if k is understood) we denote the set of matrices of order k the first $2k - 1 - m$ perdiagonals of which vanish (i.e., only the last m perdiagonals may contain nonzero elements). We now have the following result.

THEOREM 1. *Let a proper lower Hessenberg matrix J and vectors $\mathbf{c} = (c_1, c_2, \ldots, c_k)^T$ and $\mathbf{u}$ be given. Then there is at most one symmetric tridiagonal matrix $\tilde{J}$ and lower triangular matrix L satisfying (2.2) and such that $L\mathbf{e}_1 = \mathbf{u}$. Furthermore, if J is also tridiagonal, then for $i \geqslant 0$ the first $k+i$ perdiagonals of L and the first $k+i-1$ perdiagonals of $\tilde{J}$ are independent of the trailing elements $c_{i+1}, c_{i+2}, \ldots, c_k$.*

Proof. Denoting by $\tilde{\beta}_0 = 1$, $\mathbf{v}_j = \beta_{j-1} L\mathbf{e}_j$ the scaled columns of L and $\tilde{J}$ as in the output of Algorithm 1, the equation (2.2) can be rewritten as

$$\begin{aligned} J\mathbf{v}_j &= \tilde{\beta}_{j-1}\left(L\tilde{J} - \mathbf{e}_k \mathbf{c}^T\right)\mathbf{e}_j \\ &= \tilde{\beta}_{j-1}\mathbf{v}_{j+1} + \tilde{\alpha}_j \mathbf{v}_j + \frac{\tilde{\beta}_{j-1}^2}{\tilde{\beta}_{j-2}}\mathbf{v}_{j-1} - \tilde{\beta}_{j-1} c_j \mathbf{e}_k, \\ & \qquad j = 1, 2, \ldots, k \quad (\text{with } \mathbf{v}_0 = \mathbf{v}_{k+1} = \mathbf{0}). \end{aligned} \tag{2.4}$$

Like the Lanczos method, Algorithm 1 is an explicit inductive construction of the columns $\mathbf{v}_2, \ldots, \mathbf{v}_k$ and elements of $\tilde{J}$ exploiting the shape of L, i.e., using $\mathbf{e}_i^T \mathbf{v}_j = 0$ for $i < j$. This shows the uniqueness of $\tilde{J}$ (with positive $\tilde{\beta}_j$). To see the dependence on the trailing elements of the vector $\mathbf{c}$ we observe that for J tridiagonal the vector relation (2.4) considered elementwise uses the elements (i, j), $(i+1, j)$, and $(i, j-1)$ of L to determine the $(i, j+1)$st element. The c_r element of $\mathbf{c}$ is involved only for $(i, j) = (k, r)$. Furthermore, by inspecting (2.4) and Algorithm 1, the evaluation of $\tilde{\alpha}_j$ (the $2j-1$st perdiagonal of $\tilde{J}$) involves the $(j+1, j)$ element (the $2j$th perdiagonal) of L, while $\tilde{\beta}_j$ (the $2j$th perdiagonal of $\tilde{J}$) using γ_{j+1} needs the $(j+1, j+1)$ element (the $2j+1$st perdiagonal) of L. ■

In [9] we have reviewed, using the matrix notation, some classical results concerning orthogonal polynomials, which we now repeat without proof.

LEMMA 2. *If the polynomial base $\mathbf{p}, p_k$ is orthonormal on an interval (a, b) with respect to a function w, i.e. if*

$$\int_a^b p_k \mathbf{p} w = \mathbf{0}, \qquad \int_a^b p_k^2 w = 1, \tag{2.5}$$

and

$$\int_a^b \mathbf{p}\mathbf{p}^T w = I, \tag{2.6}$$

then the matrix J from the identity (2.1) *is a symmetric tridiagonal matrix* (*called the* Jacobi matrix *corresponding to the weight function w*) *satisfying*

$$J = \int_a^b t\,\mathbf{p}(t)\mathbf{p}^T(t)w(t)\,dt. \tag{2.7}$$

The following result is used in many, if not most, methods for calculating Jacobi matrices.

THEOREM 2. *Using the notation of Lemma* 1, *let the basis $\tilde{\mathbf{p}}, \tilde{p}_k$ be orthonormal on (a,b) with respect to a function $\tilde{w}$. Denote*

$$M := \int_a^b \mathbf{p}\mathbf{p}^T\tilde{w}, \qquad M_1 := \int_a^b t\,\mathbf{p}(t)\mathbf{p}^T(t)\tilde{w}(t)\,dt \tag{2.8}$$

Then

$$M = LL^T, \tag{2.9}$$

where L satisfies (2.3a) *and the Jacobi matrix for $\tilde{w}$ satisfies*

$$\tilde{J} = L^{-1}M_1L^{-T}. \tag{2.10}$$

Proof. The proof of both (2.9) and (2.10) follows immediately by substituting (2.3a) into the definitions of M (2.8) and $\tilde{J}$ [analogous to (2.7)], respectively. ∎

Note that we do not need the orthonormality of the basis $\mathbf{p}$, p_k in Theorem 2. Choosing, for example $p_j(t) := t^j$, $j = 0, 1, \ldots,$ the matrices M and M_1 are the matrices of *standard moments* of $\tilde{w}$. $\tilde{J}$ is then obtained from (2.10) by (inverse) Cholesky decomposition (2.9). The severe numerical instability of this approach may be lessened by choosing a better $\mathbf{p}$, p_k, usually orthonormal with respect to some weight function w, for which the matrices M and M_1, of *modified moments*, are explicitly known or can be efficiently calculated (see [3], [4], [5]).

Our first aim is to study the situation when the basis $\mathbf{p}$, p_k *is* orthonormal with respect to a weight function w (for which the Jacobi matrix J is known) *and* when the two weight functions w and $\tilde{w}$ satisfy

$$\tilde{w} = rw \tag{2.11}$$

where r is a polynomial of degree m.

The next result is essentially equivalent to Theorem 5 in [9].

THEOREM 3. *Let J and $\tilde{J}$ be the Jacobi matrices of order k corresponding respectively to the weight functions w and $\tilde{w}$ satisfying* (2.11) *where $m < k$. Let L and $\mathbf{c}$ satisfy* (2.2). *Then the first $k - m$ elements of $\mathbf{c}$ vanish.*

Proof. By (2.3b) and orthonormality of $\tilde{\mathbf{p}}$ we have

$$\mathbf{c}^T = \int_a^b \left(\beta_k p_k - \tilde{\beta}_k \tilde{p}_k \mathbf{e}_k^T L \mathbf{e}_k\right)\tilde{\mathbf{p}}^T \tilde{w}$$

$$= \beta_k \int_a^b p_k \mathbf{p}^T r w L^{-T},$$

from which the result follows considering the degree of the polynomial r and orthogonality of p_k and noting that L^{-T} is upper triangular. ∎

The next lemma lists some properties of matrices with vanishing perdiagonals.

LEMMA 3. *If J is lower Hessenberg, L lower triangular, and $Z \in \mathbb{Z}_m$, then Z^T, LZ, $ZL^T \in \mathbb{Z}_m$ and $JZ \in \mathbb{Z}_{m+1}$. Furthermore, if $\tilde{L}$ is another lower triangular matrix such that $LL^T - \tilde{L}\tilde{L}^T \in \mathbb{Z}_m$, then $L - \tilde{L} \in \mathbb{Z}_m$.*

Proof. Straightforward by inspection; the last statement follows from the construction of the Cholesky decomposition. ∎

The last result of this section generalizes (2.7) of Lemma 2.

THEOREM 4. *Let $\mathbf{p}$ be orthonormal with respect to w, and r a polynomial of degree m. Then*

$$\int_a^b r\mathbf{p}\mathbf{p}^T w - r(J) \in \mathbb{Z}_{m-1}, \tag{2.12}$$

where J is the Jacobi matrix corresponding to w.

Proof. To prove (2.12) it is sufficient to show that

$$\int_a^b t^j \mathbf{p}(t)\mathbf{p}^T(t) w(t)\, dt - J^j \in \mathbb{Z}_{j-1} \tag{2.13}$$

for $j = 0, 1, \dots, m$. This is obvious for $j = 0$ and $j = 1$. For the induction step, assuming $J^j = \int_a^b t^j \mathbf{p}\mathbf{p}^T w + Z_{j-1}$, $Z_{j-1} \in \mathbf{Z}_{j-1}$, we have $J^{j+1} = X + JZ_{j-1}$, where $JZ_{j-1} \in \mathbf{Z}_j$ by Lemma 3 and

$$X := \int_a^b t^j J \mathbf{p}\mathbf{p}^T w = \int_a^b t^{j+1} \mathbf{p}\mathbf{p}^T w - Y,$$

in which [by the identity (2.1)]

$$Y := \beta_k \mathbf{e}_k \int_a^b t^j p_k(t) \mathbf{p}^T(t) w(t)\, dt \in \mathbf{Z}_j$$

by the orthonormality of p_k. ■

3. MAIN RESULTS

When L_1 is any nonsingular lower triangular matrix, the matrix $J_1 := L_1^{-1} J L_1$ is similar to J. If L_1 is the Cholesky decomposition of $J - \alpha I = L_1 L_1^T$, we have also $J_1 = L_1^T L_1 + \alpha I$ (one step of the symmetric LR method), In [9] we have shown that if J is the Jacobi matrix for w, then this J_1 is, but for the last row and column, the Jacobi matrix for $\tilde{w}(t) = (t-\alpha) w(t)$. The following result generalizes this symmetric LR transformation for modifications by polynomials of arbitrary degree.

THEOREM 5. *Let r be a polynomial of degree $m < k$ such that the Cholesky decomposition*

$$r(J) = L_1 L_1^T \tag{3.1}$$

exists (i.e. $r(\lambda) > 0$ for any eigenvalue λ of J). Then, denoting $J_1 := L_1^{-1} J L_1$ and $B = J\{r(J)\}^{-1}$,

(i) *B is symmetric and $B = r(J)^{-1} J$,*
(ii) *$J_1 = L_1^T B L_1$,*
(iii) *J_1 is a symmetric tridiagonal matrix,*
(iv) *$\tilde{J} - J_1 \in \mathbf{Z}_m$, where $\tilde{J}$ is the Jacobi matrix for $\tilde{w} = rw$.*

Proof. As J is symmetric, there exist matrices Q (orthogonal) and Λ (diagonal) such that $J = Q\Lambda Q^T$. The matrix B is then

$$B = Q\Lambda\{r(\Lambda)\}^{-1} Q^T = Q\{r(\Lambda)\}^{-1} \Lambda Q^T, \tag{3.2}$$

as diagonal matrices commute. This proves (i) as well as (ii) by simple substitution from (3.1). J_1 is lower Hessenberg by definition; its symmetry follows from (ii) because B is symmetric—therefore J_1 is also tridiagonal. Finally, using (2.9), (2.12), (3.1), and Lemma 3, we obtain $L - L_1 \in \mathbf{Z}_{m-1}$ and, in particular, $L\mathbf{e}_1 = L_1\mathbf{e}_1$ because $k > m$. By definition, matrix J_1 satisfies $L_1 J_1 = JL_1$, which is (2.2) with $\mathbf{c} = \mathbf{0}$ and L replaced by L_1. However, by Theorem 3, $\mathbf{c} = 0$ except for the last m elements, and (iv) follows from Theorem 1, which asserts that given the first column of L and the first $m - k$ elements of $\mathbf{c}$, the solution $\tilde{J}$ of (2.2) is uniquely determined up to the last m perdiagonals. ∎

A similarity transformation does not change the eigenvalues of a matrix. However, Theorem 5 tells us how a *particular* similarity transformation of Jacobi matrices changes the eigenvalues of *principal submatrices* of certain orders—to the roots of polynomials orthogonal with respect to a new weight function related to the choice of the similarity transformation. In what follows we shall derive two reformulations of Theorem 5, important for deriving numerical methods implementing these transformations as well as for emphasizing their relation to the similarity transformations used in LR and QR methods for the evaluation of eigenvalues.

Given some shift α and a scalar $\sigma \neq 0$, we may consider a decomposition

$$\sigma(J - \alpha I) = XR \tag{3.3}$$

where R is an upper triangular matrix. The matrix

$$\hat{J} := \frac{1}{\sigma} RX + \alpha I \tag{3.4}$$

is then similar to J because $\hat{J} = X^{-1}JX = RJR^{-1}$ (we may require either of the matrices in the decomposition to be nonsingular). As the matrix J_1 of Theorem 5 also satisfies $J_1 = L_1^T J L_1^{-T}$ (a direct consequence of J and J_1 being symmetric), it is interesting to note what condition we need to impose on X to make $R = L_1^T$ and thus $\hat{J} = J_1$.

Corollary 1. *If R and X are nonsingular and*

$$XX^T = \sigma^2(J - \alpha I)\{r(J)\}^{-1}(J - \alpha I), \tag{3.5}$$

then the XR transformation (3.3), (3.4) *results in modifying the Jacobi matrix J by polynomial r, i.e., $\hat{J} = J_1$ of Theorem* 5.

Proof. From (3.5) and (3.3) we have (J being symmetric)

$$XX^T = XR\{r(J)\}^{-1}R^TX^T,$$

and $R = L_1^T$ follows from the uniqueness of the Cholesky decomposition. ■

Applying this result to the case $r(t) := \sigma(t-\alpha)$, σ of suitable sign, the relation (3.5) becomes $XX^T = \sigma(J - \alpha I)$, i.e. equivalent to (3.3) if we choose $X = R^T = L_1$—the symmetric LR transformation with a shift.

Similarly, in the case $r(t) := \sigma^2(t-\alpha)^2$ the matrix X is required, by (3.5), to be orthogonal—the QR transformation with a shift. This result is slightly stronger than the one in [9], as we need to discard only the last two perdiagonals in J_1, that is, the last *one* rather than *two* rows and columns, to obtain the correct $\tilde{J}$.

For other polynomials r the requirement (3.5) is not simple any more. However, we can proceed in the following way. Let, as in the proof of Theorem 5,

$$J = Q\Lambda Q^T \tag{3.6}$$

be the diagonalization of the Jacobi matrix J, and denote

$$D^2 := r(\Lambda) \tag{3.7}$$

[all diagonal elements of $r(\Lambda)$ are positive by the assumption in Theorem 5] and $\Lambda_\alpha := \Lambda - \alpha I$ (assumed nonsingular). For (3.5) to hold we must have

$$Q^TXX^TQ = \sigma^2\Lambda_\alpha D^{-2}\Lambda_\alpha,$$

which implies that matrix $U := (1/\sigma)D\Lambda_\alpha^{-1}Q^TX$ must be orthogonal. Because the relation (3.3) implies $Q^TXR = \sigma\Lambda_\alpha Q^T$, we have

$$UR = DQ^T, \tag{3.8}$$

and U and R can thus be obtained by the QR decomposition of a known matrix. As $X = \sigma Q\Lambda_\alpha D^{-1}U$, we have

$$J_1 = \hat{J} = X^{-1}JX = U^TD\Lambda_\alpha^{-1}Q^TJQ\Lambda_\alpha D^{-1}U = U^T\Lambda U.$$

We have thus proved the following result.

COROLLARY 2. *The modification of the Jacobi matrix by a polynomial r satisfying the assumptions of Theorem* 5 *can be achieved by the QR decomposition* (3.8) *and by constructing*

$$J_1 = U^T \Lambda U. \tag{3.9}$$

The last result allows us to comment on reversing this process, that is, on modification of a Jacobi matrix by dividing, rather than multiplying, its weight function by a given polynomial r. In other words, given $\tilde{J}$ and r, how can we find J from (3.6), (3.7), (3.8), and (3.9) where we know, by Theorem 5, that $Z_m := J_1 - \tilde{J} \in \mathbf{Z}_m$? We observe that to obtain J from J_1 involves exactly the same steps as to obtain J_1 from J: diagonalize J_1 to find Λ, U^T in (3.9), compute $D^{-1} = r(\Lambda)^{-2}$, find the QR decomposition of $D^{-1}U = Q^T R^{-1}$ [as from (3.8)], and finally construct $J = Q \Lambda Q^T$. However, to obtain $J_1 = \tilde{J} + Z_m$ we need the m nonzero elements on the diagonal and subdiagonal of Z_m. In fact, additional information about the weight function $\tilde{w}$ is needed to determine such a modification uniquely—we intend to treat this problem in another paper.

In some applications involving Jacobi matrices the first moment $\mu_0 = \int_a^b w$ of the weight function is needed. It is therefore useful to know how to obtain the first moment of the modified weight function $\tilde{w}$. As, by orthonormality, $\mu_0 p_0^2 = 1$ and $\mathbf{p} = L\tilde{\mathbf{p}}$ [see (2.3a)], we have immediately

$$\tilde{\mu}_0 := \int_a^b \tilde{w} = \left(\mathbf{e}_1^T L \mathbf{e}_1\right)^2 \mu_0. \tag{3.10}$$

Here the matrix L may be replaced by the matrix L_1 of Theorem 5 or the matrices R in Corollaries 1 and 2.

4. METHODS

In this section we will describe several methods implementing the results of the previous section. In all of them, the input is (1) the Jacobi matrix J of order n for some weight function w, and (2) the polynomial r of given degree m. The output is (1) the Jacobi matrix $\tilde{J}$, of order $\tilde{n} = n - [m/2] - 1$, for the weight function $\tilde{w} = rw$, and (2) the parameter $\rho = \tilde{\mu}_0/\mu_0$ for the modification of the first moment. The methods may differ in the way the polynomial r is specified. As we mentioned in the introduction, r could be given, implicitly, as a polynomial approximation to the given function $\tilde{w}/w$. However, we shall first discuss two methods for the case where the polynomial r is available for point evaluation. We shall also mention, mainly for reasons of comparison and testing, a method based on the explicit knowledge of the roots of r.

Method 1: "LT Lanczos"

We note that Algorithm 1 of Section 2, given J and $\mathbf{c} := 0$, finds a tridiagonal matrix J_1 [compare (2.2), Theorem 5, and the proof of Theorem 5, part (iv)] satisfying

$$L_1 J_1 = J L_1 \tag{4.1}$$

as long as the first column $\mathbf{u} = L_1 \mathbf{e}_1$ of the lower triangular matrix L_1 is given. However, by (3.1), $\mathbf{u} = \mathbf{d}(\mathbf{e}_1^T \mathbf{d})^{-1/2}$, where $\mathbf{d} := r(J)\mathbf{e}_1$. We may find $\mathbf{d}$ using the diagonalization of $J = Q \Lambda Q^T$. We have then

$$\mathbf{d} = Q r(\Lambda) Q^T \mathbf{e}_1, \tag{4.2}$$

and the desired parameter ρ is $\rho = \mathbf{e}_1^T \mathbf{d}$.

As $r(J)$ is $(2m+1)$-banded, we know that $\mathbf{d}$ is $(m+1)$-banded (i.e., $\mathbf{e}_j^T \mathbf{d} = 0$ for $j > m+1$). We therefore need only the first $m+1$ rows of Q to calculate $\mathbf{d}$ by (4.2). These may be obtained, for example, by a suitable modification of the procedure IMQLT2 of [11].

Algorithm 1 is closely related to the Lanczos method, which requires the matrix L_1 in (4.1) to be orthogonal rather than lower triangular. We therefore call this process the "lower triangular Lanczos method."

Method 2: "PSI QR"

This method is the direct implementation of the Corollary 2 of Section 3 in which the QR decomposition of (3.8) is performed implicitly (see, e.g. [11] with reversed order of the rows in Q and L). This means that the orthogonal matrix U is sought in the form

$$U = H_1 H_2 \cdots H_{n-1}$$

where H_j, $j = 1, 2, \ldots, n-1$, are symmetric elementary Householder transformations. However, only H_1 is determined directly from (3.8), so that only the first row of Q is needed in the process (the factor ρ is then $\rho = \mathbf{e}_1^T Q D^2 Q^T \mathbf{e}_1$, because $R\mathbf{e}_1 = \sqrt{\rho}\,\mathbf{e}_1$ and thus $DQ^T \mathbf{e}_1 = \sqrt{\rho}\, U \mathbf{e}_1$). The other transformations are then uniquely determined, and can be calculated as in the implicit QR

method, from the requirement that the matrix

$$J_1 = U^T \Lambda U = H_{n-1} \cdots H_2 H_1 \Lambda H_1 H_2 \cdots H_{n-1}$$

should be tridiagonal.

So far we have assumed that the modifying polynomial r was positive on (a,b), or at least $r(\lambda_j) > 0$, $j = 1,2,\dots,n$, where $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$. However, with minor modifications, this method needs to assume only that $r \geq 0$ on (a,b). Such a polynomial can only have roots of even multiplicity inside (a,b), so there cannot be more than $[m/2]$ distinct roots there. Thus, the eigenvalues of J being distinct, there can be at most $[m/2]$ zero diagonal elements in D. We may choose a permutation of the columns of Q and of the diagonal elements of Λ such that these zero elements in D come last. It is easy to see that they will not affect the computation of the order $\tilde{n} = n - [m/2] - 1$ principal submatrix of J_1 which is the required $\tilde{J}$. In fact, it may be advantageous to order Λ always in terms of decreasing magnitudes of $r(\lambda_j)$.

Method 2 is based on the implicit QR transformation—where, however, the matrix D results from a polynomial evaluation of the original matrix rather than a linear shift. We thus choose to call it the polynomial shift implicit QR method.

Method 3: "LR-QR"

In this method we require the polynomial r to have real roots and be given in the form $r(t) = \Pi_{j=1}^{s}\{\sigma_j(t - v_j)\}^{m_j}$, where $m_1 + m_2 + \cdots + m_s = m$, $\sigma_j = -1$ if m_j is odd and $v_j \geq b$, and $\sigma_j = 1$ otherwise. The method then comprises a series of QR and symmetric LR transformations of the input matrix J, with appropriate shifts, as indicated in the discussion after Corollary 1 of Section 3 and as described in detail in Algorithm 1 of [9]. We note that if there are q distinct roots of r of odd multiplicity, the process requires q symmetric LR steps and $(m-q)/2$ QR steps.

Finally we wish to state, without proof, two simple results regarding the construction of polynomials approximating an arbitrary function $f := \tilde{w}/w$. In (4.2) we have shown that the trailing elements of $\mathbf{d}$ vanish if r is a polynomial. We may ask what will happen if we replace r by f in (4.2) and truncate $\mathbf{d}$, i.e. we define

$$\mathbf{d} := \left(\mathbf{d}_m^T, 0, 0, \dots, 0\right)^T,$$

where

$$\mathbf{d}_m := Q_m f(\Lambda) Q^T \mathbf{e}_1, \qquad f(\Lambda) := \mathrm{diag}(f(\lambda_1), \dots, f(\lambda_n))$$

and Q_m is the $(m+1)\times n$ matrix comprising the first $m+1$ rows of Q. It is not difficult to show that $\mathbf{d}=r(J)\mathbf{e}_1$, where r is the best w-weighted least squares fit to f evaluated by Gauss quadrature with the diagonal elements of Λ as knots. Furthermore, $r(\cdot)=(1/p_0)\mathbf{d}^T\mathbf{p}(\cdot)$, where $\mathbf{p}$ are the polynomials orthonormal with respect to w satisfying (2.1). For Method 2 we obtain the formula

$$r(\Lambda)=\{\operatorname{diag}(Q^T\mathbf{e}_1)\}^{-1}Q_m^TQ_mf(\Lambda)Q^T\mathbf{e}_1$$

because

$$\mathbf{p}(\lambda_j)=\frac{p_0Q\mathbf{e}_j}{\mathbf{e}_j^TQ^T\mathbf{e}_1}.$$

Slightly more complicated results may be obtained for least squares fits with respect to weight functions other than w. One may also consider, for greater efficiency, using Gauss quadratures with $m+1$ rather than n knots. We return to these questions in a future paper.

5. NUMERICAL TESTS

In [6] Gautschi states that his algorithm for polynomial modification, essentially equivalent—though slightly more general—to the *LR-QR* method, "appears to be numerically stable." We have made a similar observation in [9] based on the following test. Jacobi matrices $J^{(\alpha,\beta)}$ for the weight function

TABLE 1

MAXIMAL ERRORS OF DIAGONAL (E_α) AND SUBDIAGONAL (E_β) ELEMENTS OF JACOBI MATRICES MODIFIED BY VARIOUS METHODS[a]

Order of	LT Lanczos		PSI *QR*		*LR-QR*	
$\tilde{J}$	E_α	E_β	E_α	E_β	E_α	E_β
10	2.5(− 7)	4.5(− 8)	1.1(− 7)	7.1(− 8)	1.5(− 8)	7.5(− 9)
20	1.3(− 6)	8.8(− 7)	1.8(− 7)	1.2(− 7)	2.2(− 8)	1.1(− 8)
30	3.1(− 6)	2.8(− 6)	2.9(− 7)	2.9(− 7)	3.0(− 8)	1.5(− 8)
40	3.9(− 6)	9.1(− 7)	4.1(− 7)	3.4(− 7)	3.0(− 8)	1.9(− 8)
50	1.3(− 6)	2.0(− 5)	4.4(− 7)	4.7(− 7)	3.0(− 8)	1.9(− 8)
60	3.2(− 5)	2.5(− 5)	1.1(− 6)	5.9(− 7)	4.5(− 8)	1.9(− 8)
70	2.6(− 5)	1.3(− 5)	1.1(− 6)	5.8(− 7)	4.5(− 8)	1.9(− 8)

[a]Weight function $w\equiv 1$ modified by the polynomial $r(t)=(1-t^2)^2$.

$w^{(\alpha,\beta)}(t) := (1-t)^{\alpha}(1+t)^{\beta}$, $\alpha, \beta > -1$, are explicitly known. We can therefore choose $w = w^{(\alpha,\beta)}$ and check the accuracy of the modification by $r(t) = (1-t)^{\delta\alpha}(1+t)^{\delta\beta}$ for integer $\delta\alpha, \delta\beta$ by reference to the known $J^{(\alpha+\delta\alpha,\beta+\delta\beta)}$. In Tables 1 and 2 we present results of such tests performed in single precision on a DEC-10 (7 decimal digits). We table the maximal absolute errors of both the diagonal and subdiagonal elements for various orders $\tilde{n}$ of the required matrix $\tilde{J}$.

As mentioned above, the *LR-QR* method indeed demonstrates its stability—there is almost no increase in the errors over the range of $\tilde{n}$. We are, however, interested in the performance of the methods not requiring the knowledge of the roots of r. The rate of increase of the errors of the PSI *QR* method with increasing $\tilde{n}$ appears to be linear, while that of the LT Lanczos method appears exponential. For larger $\delta\alpha, \delta\beta$ the LT Lanczos method breaks down (for sufficiently large $\tilde{n}$) as, due to roundoff errors, the calculated subdiagonal elements $\tilde{\beta}_j^2$ become negative (we tabulate the index j for which this occurs). This is not surprising, as, for higher multiplicity roots at ± 1, many diagonal elements of $r(\Lambda)$ are close to zero and the matrix $r(J)$ is almost singular. The LT Lanczos method implicitly performs the Cholesky decomposition of $r(J)$, which is known to be unreliable for almost singular matrices.

In Table 3 we present errors of the two methods for the modifying polynomial $r(t) = (v-t)^{m_1}(t+v)^{m_2}$ for various values of $v \geqslant 1$. As a reference we have used the Jacobi matrix calculated in double precision by the *LR-QR* method. We observe that as the roots of the modifying polynomial move away from the support of the weight function, the performance of the

TABLE 2

MAXIMAL ERRORS OF DIAGONAL (E_α) AND SUBDIAGONAL (E_β) ELEMENTS OF JACOBI MATRICES MODIFIED BY VARIOUS METHODS[a]

	LT Lanczos[b]		PSI *QR*		*LR-QR*	
Order of $\tilde{J}$	E_α	E_β	E_α	E_β	E_α	E_β
10	4.2(−5)	7.4(−5)	9.6(−8)	6.3(−8)	3.3(−8)	1.9(−8)
20	8.8(−2)	7.3(−2)	1.1(−6)	5.8(−7)	3.8(−8)	1.9(−8)
30	6.7(−3)	7.0(−3)	9.7(−6)	5.1(−6)	3.8(−8)	2.2(−8)
40	19*		7.5(−6)	3.8(−6)	4.1(−8)	2.2(−8)
50	37*		4.4(−5)	2.3(−5)	6.0(−8)	2.2(−8)
60	26*		3.3(−4)	1.7(−4)	6.0(−8)	2.2(−8)
70	37*		9.9(−4)	5.1(−4)	6.0(−8)	2.2(−8)

[a]Weight function $w \equiv 1$ modified by the polynomial $r(t) = (1-t)^4(1+t)^5$.
[b]j^* means that method failed in the jth step.

LT Lanczos method improves markedly, whereas the PSI QR method performs well independently of the position of these roots.

Finally, we wish to observe that two close Jacobi matrices have also close eigenvalues and eigenvectors. In fact, if $\tilde{J} = J + \varepsilon E$, where $\max_{i,j}|\mathbf{e}_i^T E \mathbf{e}_j| = 1$ (E is, of course, symmetric tridiagonal), then, following [1], we have that

$$\tilde{\lambda}_i = \lambda_i + O(\varepsilon),$$
$$\tilde{\mathbf{x}}_i = \mathbf{x}_i + \mathbf{O}(\varepsilon),$$

where $\lambda_i, \mathbf{x}_i$ and $\tilde{\lambda}_i, \tilde{\mathbf{x}}_i$ are eigenpairs of J and $\tilde{J}$, respectively, and the eigenvectors are normalized. Here the $\mathbf{O}(\varepsilon)$ term for the eigenvectors depends on the closeness of the eigenvalues λ_i (always distinct in our case); however, a more careful analysis shows that

$$|\tilde{\lambda}_i - \lambda_i| \leqslant 3\varepsilon.$$

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TABLE 3

MAXIMAL ERRORS OF DIAGONAL (E_α) AND SUBDIAGONAL (E_β) ELEMENTS OF JACOBI MATRICES MODIFIED BY VARIOUS METHODS[a]

	LT Lanczos[b]		PSI QR		LR-QR	
v	E_α	E_β	E_α	E_β	E_α	E_β
1.00	19*		7.5(−6)	3.8(−6)	6.3(−8)	2.6(−8)
1.01	22*		1.9(−5)	9.5(−6)	4.4(−8)	2.2(−8)
1.02	29*		1.5(−6)	6.9(−7)	3.9(−8)	2.6(−8)
1.025	3.3(−2)	2.2(−2)	1.2(−6)	6.0(−7)	5.1(−8)	2.6(−8)
1.03	1.4(−3)	6.8(−4)	1.5(−6)	7.1(−7)	3.7(−8)	2.2(−8)
1.10	1.2(−5)	5.9(−6)	4.7(−7)	1.5(−7)	4.8(−8)	2.2(−8)
1.50	1.1(−7)	6.7(−8)	3.1(−7)	3.1(−7)	7.2(−8)	2.2(−8)
2.00	3.5(−8)	1.5(−8)	4.7(−7)	2.8(−7)	8.3(−8)	3.0(−8)
4.00	3.7(−8)	7.5(−9)	3.1(−7)	1.3(−7)	1.8(−7)	3.7(−8)
10.00	3.9(−8)	7.5(−9)	3.1(−7)	2.3(−7)	7.5(−7)	6.7(−8)

[a]Weight function $w \equiv 1$ modified by the polynomial $r(t) = (v-t)^4 (v+t)^5$. Order of $\tilde{J}$ is 40.

[b]j^* means that method failed in the jth step.

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