Calculation of Gauss Quadrature Rules*

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Abstract. Several algorithms are given and compared for computing Gauss quadrature rules. It is shown that given the three term recurrence relation for the orthogonal polynomials generated by the weight function, the quadrature rule may be generated by computing the eigenvalues and first component of the orthornormalized eigenvectors of a symmetric tridiagonal matrix. An algorithm is also presented for computing the three term recurrence relation from the moments of the weight function. ■

Introduction. Most numerical integration techniques consist of approximating the integrand by a polynomial in a region or regions and then integrating the polynomial exactly. Often a complicated integrand can be factored into a non-negative "weight" function and another function better approximated by a polynomial, thus

$$\int_a^b g(t)dt = \int_a^b \omega(t)f(t)dt \approx \sum_{j=1}^{N} w_j f(t_j) .$$

Hopefully, the quadrature rule $\{w_j, t_j\}_{j=1}^{N}$ corresponding to the weight function $\omega(t)$ is available in tabulated form, but more likely it is not. We present here two algorithms for generating the Gaussian quadrature rule defined by the weight function when:

(a) the three term recurrence relation is known for the orthogonal polynomials generated by $\omega(t)$, and

(b) the moments of the weight function are known or can be calculated.

In [6], Gautschi presents an algorithm for calculating Gauss quadrature rules when neither the recurrence relationship nor the moments are known.

1. Definitions and Preliminaries. Let $\omega(x) \geqq 0$ be a fixed *weight function* defined on $[a, b]$. For $\omega(x)$, it is possible to define a sequence of polynomials $p_0(x), p_1(x), \cdots$ which are orthonormal with respect to $\omega(x)$ and in which $p_n(x)$ is of exact degree n so that

$$\int_a^b \omega(x)p_m(x)p_n(x)dx = 1 \quad \text{when } m = n ,$$
$$= 0 \quad \text{when } m \neq n . \tag{1.1}$$

The polynomial $p_n(x) = k_n \prod_{i=1}^{n} (x - t_i)$, $k_n > 0$, has n real roots $a < t_1 < t_2 <$

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$\cdots < t_n < b$. The roots of the orthogonal polynomials play an important role in Gaussian quadrature.

THEOREM. *Let* $f(x) \in C^{2N}[a, b]$, *then*

$$\int_a^b \omega(x) f(x) dx = \sum_{j=1}^{N} w_j f(t_j) + \frac{f^{(2N)}(\xi)}{(2N)! k_N{}^2}, \qquad (a < \xi < b),$$

where

$$w_j = -\frac{k_{N+1}}{k_N} \frac{1}{p_{N+1}(t_j) p_N'(t_j)}, \quad \left(p_N'(t_j) = \frac{dp_N(t)}{dt}\bigg|_{t=t_j}\right), \qquad j = 1, 2, \cdots, N.$$

Thus the Gauss quadrature rule is exact for all polynomials of degree $\leqq 2N - 1$.

Proofs of the above statements and Theorem can be found in Davis and Rabinowitz [4, Chapter 2].

Several algorithms have been proposed for calculating $\{w_j, t_j\}_{j=1}^{N}$; cf. [10], [11]. In this note, we shall give effective numerical algorithms which are based on determining the eigenvalues and the first component of the eigenvectors of a symmetric tridiagonal matrix.

2. Generating the Gauss Rule. Any set of orthogonal polynomials, $\{p_j(x)\}_{j=1}^{N}$, satisfies a three term recurrence relationship:

$$p_j(x) = (a_j x + b_j) p_{j-1}(x) - c_j p_{j-2}(x), \qquad (2.1)$$
$$j = 1, 2, \cdots, N; \quad p_{-1}(x) \equiv 0, \quad p_0(x) \equiv 1,$$

with $a_j > 0$, $c_j > 0$. The coefficients $\{a_j, b_j, c_j\}$ have been tabulated for a number of weight functions $\omega(x)$, cf. [8]. In Section 4 we shall give a simple method for generating $\{a_j, b_j, c_j\}$ for any weight function.

Following Wilf [12], we may identify (2.1) with the matrix equation

$$x \begin{bmatrix} p_0(x) \\ p_1(x) \\ \cdot \\ \cdot \\ \cdot \\ p_{N-1}(x) \end{bmatrix} = \begin{bmatrix} -b_1/a_1, & 1/a_1, & 0 & & & \\ c_2/a_2, & -b_2/a_2, & 1/a_2 & & & \\ 0 & \cdot & \cdot & \cdot & & \\ & & \cdot & \cdot & \cdot & \\ & & & \cdot & \cdot & 1/a_{N-1} \\ & & & & c_N/a_N, & -b_N/a_N \end{bmatrix} \begin{bmatrix} p_0(x) \\ p_1(x) \\ \cdot \\ \cdot \\ \cdot \\ p_{N-1}(x) \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ \cdot \\ \cdot \\ 0 \\ p_N(x)/a_N \end{bmatrix}$$

or, equivalently in matrix notation

$$x\mathbf{p}(x) = T\mathbf{p}(x) + (1/a_N)p_N(x)\mathbf{e}_N$$

where T is the tridiagonal matrix and $\mathbf{e}_N = (0, 0, \cdots, 0, 1)^T$. Thus $p_N(t_j) = 0$ if and only if $t_j\mathbf{p}(t_j) = T\mathbf{p}(t_j)$ where t_j is an eigenvalue of the tridiagonal matrix T. In [12], it is shown that T is symmetric if the polynomials are orthonormal. If T is not symmetric, then we may perform a diagonal similarity transformation which will yield a symmetric tridiagonal matrix J. Thus

$$DTD^{-1} = J = \begin{bmatrix} \alpha_1 & \beta_1 & 0 & & & \\ \beta_1 & \alpha_2 & \beta_2 & & & \\ 0 & \cdot & \cdot & \cdot & & \\ & & \cdot & \cdot & \cdot & \\ & & & \cdot & \cdot & \beta_{N-1} \\ & & & & \beta_{N-1} & \alpha_N \end{bmatrix}$$

where

$$\alpha_i = -\frac{b_i}{a_i}, \quad \beta_i = \left(\frac{c_{i+1}}{a_i a_{i+1}}\right)^{1/2}. \tag{2.2}$$

It is shown by Wilf [12] that as a consequence of the Christoffel-Darboux identity

$$w_j[\mathbf{p}(t_j)]^T[\mathbf{p}(t_j)] = 1, \qquad j = 1, 2, \cdots, N \tag{2.3}$$

where $\mathbf{p}(t_j)$ corresponds to the eigenvector associated with the eigenvalue t_j. Suppose that the eigenvectors of T are calculated so that

$$J\mathbf{q}_j = t_j\mathbf{q}_j, \qquad j = 1, 2, \cdots, N \tag{2.4}$$

with $\mathbf{q}_j{}^T\mathbf{q}_j = 1$. If

$$\mathbf{q}_j{}^T = (q_{1,j}, q_{2,j}, \cdots, q_{N,j}), \tag{2.5}$$

then $q_{1,j}^2 = w_j(p_0(t_j))^2$ by (2.3). Thus from (1.1), we see

$$w_j = \frac{q_{1,j}^2}{p_0{}^2(t_j)} = \frac{q_{1,j}^2}{k_0{}^2} = q_{1,j}^2 \times \int_a^b \omega(x)dx \equiv q_{1,j}^2 \times \mu_0. \tag{2.6}$$

Consequently, if one can compute the eigenvalues of T and the first component of the orthonormal eigenvectors, one is able to determine the Gauss quadrature rule.

3. The Q-R Algorithm. One of the most effective methods of computing the eigenvalues and eigenvectors of a symmetric matrix is the Q-R algorithm of Francis [5]. The Q-R algorithm proceeds as follows:

Begin with the given matrix $J = J^{(0)}$, compute the factorization $J^{(0)} = Q^{(0)}R^{(0)}$ where $Q^{(0)T}Q^{(0)} = I$ and $R^{(0)}$ is an upper triangular matrix, and then multiply the matrices in reverse order so that

$$J^{(1)} = R^{(0)}Q^{(0)} = Q^{(0)^T}J^{(0)}Q^{(0)}.$$

Now one treats the matrix $J^{(1)}$ in the same fashion as the matrix $J^{(0)}$, and a sequence of matrices is obtained by continuing *ad infinitum*. Thus

$$\begin{aligned} J^{(i)} &= Q^{(i)}R^{(i)}, \\ J^{(i+1)} &= R^{(i)}Q^{(i)} = Q^{(i+1)}R^{(i+1)} \end{aligned} \tag{3.1}$$

so that

$$J^{(i+1)} = Q^{(i)^T}J^{(i)}Q^{(i)} = Q^{(i)^T}Q^{(i-1)^T}\cdots Q^{(0)^T}JQ^{(0)}Q^{(1)}\cdots Q^{(i)}. \tag{3.2}$$

Since the eigenvalues of J are distinct and real for orthogonal polynomials, a real translation parameter λ may be chosen so that the eigenvalues of $J^{(i)} - \lambda I$ are distinct in modulus. Under these conditions, it is well known [5] that $J^{(i)} - \lambda I$ converges to the diagonal matrix of eigenvalues of $J - \lambda I$ as $i \to \infty$ and that $P^{(i)} = Q^{(0)} \times Q^{(1)} \times \cdots \times Q^{(i)}$ converges to the orthogonal matrix of eigenvectors of J. The method has the advantage that the matrix $J^{(i)} - \lambda I$ remains tridiagonal throughout the computation.

Francis has shown that it is not necessary to compute the decomposition (3.1) explicitly but it is possible to do the calculation (3.2) directly. Let

$$\{S^{(i)}\}_{k,1} = \{Q^{(i)}\}_{k,1} \qquad (k = 1, 2, \cdots, N),$$

(i.e., the elements of the first column of $S^{(i)}$ are equal to the elements of the first column of $Q^{(i)}$). Then if

(i) $K^{(i+1)} = S^{(i)^T}J^{(i)}S^{(i)}$,

(ii) $K^{(i+1)}$ is a tridiagonal matrix,

(iii) $J^{(i)}$ is nonsingular,

(iv) the subdiagonal elements of $K^{(i+1)}$ are positive, it follows that $K^{(i+1)} = J^{(i+1)}$.

For the tridiagonal matrices, the calculation is quite simple. Dropping the iteration counter i, let

$$Z_p = \begin{array}{c} \\ \\ \\ \\ \\ (p) \\ (p+1) \\ \\ \\ \\ \end{array} \begin{array}{c} \begin{array}{ccccccccccc} & & & & (p) & (p+1) & & & & & \end{array} \\ \begin{bmatrix} 1 & & & & \cdot & \cdot & & & & & \\ & \cdot & & & \cdot & \cdot & & & \bigcirc & & \\ & & \cdot & & \cdot & \cdot & & & & & \\ & & & 1 & \cdot & \cdot & & & & & \\ \cdot & \cdot & \cdot & \cdot & \cos\theta_p & \sin\theta_p & \cdot & \cdot & \cdot & \cdot & \\ & & & & & & & & & & \\ \cdot & \cdot & \cdot & \cdot & \sin\theta_p & -\cos\theta_p & \cdot & \cdot & \cdot & \cdot & \\ & & & & \cdot & \cdot & 1 & & & & \\ & \bigcirc & & & \cdot & \cdot & & \cdot & & & \\ & & & & \cdot & \cdot & & & \cdot & & \\ & & & & \cdot & \cdot & & & & 1 & \end{bmatrix} \end{array}.$$

Then $\cos\theta_1$ is chosen so that

$$\{Z_1J\}_{k,1} = 0, \qquad k = 2, 3, \cdots, N.$$

Let

$$J = \begin{bmatrix} a_1 & b_1 & 0 & & & \\ b_1 & a_2 & b_2 & & & \\ 0 & \cdot & \cdot & \cdot & & \\ & & \cdot & \cdot & \cdot & \\ & & & \cdot & \cdot & b_{N-1} \\ & & & & b_{N-1} & a_N \end{bmatrix}.$$

The matrix

$$Z_1 J Z_1 = \begin{bmatrix} a_1' & b_1' & d_1 & & & \\ b_1' & a_2' & b_2' & 0 & & \\ d_1 & b_2' & a_3 & b_3 & & \\ & 0 & b_3 & \cdot & \cdot & \\ & & & \cdot & \cdot & \cdot \\ & & & & \cdot & b_{N-1} \\ & & & & b_{N-1} & a_N \end{bmatrix},$$

where the primes indicate altered elements of J; then

$$K = Z_{N-1} Z_{N-2} \cdots Z_1 J Z_1 \cdots Z_{N-1}$$

and $Z_2, \cdots, Z_{N-1}$ are constructed so that K is tridiagonal. The product of all the orthogonal rotations yields the matrix of orthogonal eigenvectors. To determine $\{w_j\}_{j=1}^N$, however, we need only the first component of the orthonormal eigenvector. Thus, using (2.3)

$$\mathbf{q}^T \equiv [q_{1,1}, q_{1,2}, \cdots, q_{1,N}] = [1, 0, 0, \cdots, 0] \times \prod_{i=0}^{\infty} (Z_1^{(i)} \times Z_2^{(i)} \times \cdots \times Z_{N-1}^{(i)})$$

and it is not necessary to compute the entire matrix of eigenvectors. More explicitly, for $j = 1, 2, \cdots, N-1$

$$\begin{aligned}
\sin\theta_j^{(i)} &= d_{j-1}^{(i)} / [(d_{j-1}^{(i)})^2 + (\bar{b}_{j-1}^{(i)})^2]^{1/2}, \\
\cos\theta_j^{(i)} &= \bar{b}_{j-1}^{(i)} / [(d_{j-1}^{(i)})^2 + (\bar{b}_{j-1}^{(i)})^2]^{1/2}, \\
a_j^{(i+1)} &= \bar{a}_j^{(i)} \cos^2\theta_j^{(i)} + 2\tilde{b}_j^{(i)} \cos\theta_j^{(i)} \sin\theta_j^{(i)} + a_{j+1}^{(i)} \sin^2\theta_j^{(i)}, \\
\bar{a}_{j+1}^{(i)} &= \bar{a}_j^{(i)} \sin^2\theta_j^{(i)} - 2\tilde{b}_j^{(i)} \cos\theta_j^{(i)} \sin\theta_j^{(i)} + a_{j+1}^{(i)} \cos^2\theta_j^{(i)}, \\
b_{j-1}^{(i+1)} &= \bar{b}_{j-1}^{(i)} \cos\theta_j^{(i)} + d_{j-1}^{(i)} \sin\theta_j^{(i)} = [(\bar{b}_{j-1}^{(i)})^2 + (d_{j-1}^{(i)})^2]^{1/2}, \\
\bar{b}_j^{(i)} &= (\bar{a}_j^{(i)} - a_{j+1}^{(i)}) \sin\theta_j^{(i)} \cos\theta_j^{(i)} + \tilde{b}_j^{(i)} (\sin^2\theta_j^{(i)} - \cos^2\theta_j^{(i)}), \\
\tilde{b}_{j+1}^{(i)} &= -b_{j+1}^{(i)} \cos\theta_j^{(i)}, \\
d_j^{(i)} &= b_{j+1}^{(i)} \sin\theta_j^{(i)}, \; z_j^{(i+1)} = \bar{z}_j^{(i)} \cos\theta_j + z_{j+1}^{(i)} \sin\theta_j, \\
\bar{z}_{j+1}^{(i)} &= \bar{z}_j^{(i)} \sin\theta_j^{(i)} - z_{j+1}^{(i)} \cos\theta_j^{(i)},
\end{aligned} \tag{3.3}$$

with

$$\begin{aligned}
d_0^{(i)} &= b_1^{(i)}, \quad \bar{b}_0^{(i)} = (a_1^{(i)} - \lambda^{(i)}), \\
\bar{a}_1^{(i)} &= a_1^{(i)}, \quad \tilde{b}_1^{(i)} = b_1^{(i)}, \quad \bar{z}_1^{(i)} = z_1^{(i)}.
\end{aligned}$$

Initially

$$z_1^{(0)} = 1, \quad z_j^{(0)} = 0 \quad \text{for } j = 2, \cdots, N$$

so that $\mathbf{z}^{(i)T} \to \mathbf{q}^T$ as $i \to \infty$. In the actual computation, no additional storage is required for $\{\bar{a}_j^{(i)}, \bar{b}_j^{(i)}, \bar{\bar{b}}_j^{(i)}, \bar{z}_j^{(i)}\}$ since they may overwrite $\{a_j^{(i)}, b_j^{(i)}, z_j^{(i)}\}$. We choose $\lambda^{(i)}$ as an approximation to an eigenvalue; usually, it is related to the eigenvalues of the matrix

$$\begin{bmatrix} a_{N-1}^{(i)} & b_{N-1}^{(i)} \\ b_{N-1}^{(i)} & a_N^{(i)} \end{bmatrix}.$$

When $b_{N-1}^{(i)}$ is sufficiently small, $a_N^{(i)}$ is taken as eigenvalue and N is replaced by $N - 1$.

4. Determining the Three Term Relationship from the Moments. For many weight functions, the three term relationship of the orthogonal polynomials have been determined. In some situations, however, the weight function is not known explicitly, but one has a set of $2N + 1$ moments, viz.

$$\mu_k = \int_a^b \omega(x) x^k dx \qquad k = 0, 1, \cdots, 2N .$$

Based on an elegant paper of Mysovskih [9], Gautschi*** has given a simple derivation of the three term relationship which we give below. This result also follows from certain determinantal relations (cf. [7]).

Let $\Omega \subset E^n$ be a domain in n-dimensional Euclidean space and $\omega(\mathbf{x}) \geqq 0$ be a weight function on Ω for which all "moments"

$$\mu_{\gamma_1,\gamma_2,\ldots,\gamma_n} = \int_\Omega \omega(\mathbf{x}) x_1^{\gamma_1} x_2^{\gamma_2} \cdots x_n^{\gamma_n} d\mathbf{x}$$

exist, and $\mu_{0,0,\ldots,0} > 0$. Enumerate the monomials

$$x_1^{\gamma_1} x_2^{\gamma_2} \cdots x_n^{\gamma_n}, \quad \gamma_1 \geqq 0, \cdots, \gamma_n \geqq 0$$

as $\{\varphi_i(\mathbf{x})\}_{i=1}^L$, whereby $i < j$ if degree $\varphi_i <$ degree φ_j, the enumeration within the same degree being arbitrary. In particular, $\varphi_1(\mathbf{x}) = 1$. Let

$$M = [(\varphi_i, \varphi_j)]_{i,j=1}^L \equiv \{m_{ij}\}$$

denote the "Gram matrix" for the system $\{\varphi_i(\mathbf{x})\}_{i=1}^L$, where

$$(\varphi_i, \varphi_j) = \int_\Omega \omega(\mathbf{x}) \varphi_i(\mathbf{x}) \varphi_j(\mathbf{x}) d\mathbf{x} .$$

Note M is positive definite. Let $M = R^T R$ be the Cholesky decomposition of M with

$$r_{ii} = \left(m_{ii} - \sum_{k=1}^{i-1} r_{ki}^2 \right)^{1/2}$$

and

$$r_{ij} = \left(m_{ij} - \sum_{k=1}^{i-1} r_{ki} r_{kj} \right) \Big/ r_{ii} , \qquad i < j \tag{4.1}$$

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for i and j between 1 and L. Let

$$R^{-1} \equiv \begin{bmatrix} s_{11} & s_{12} & \cdot & \cdot & \cdot & s_{1L} \\ & s_{22} & \cdot & \cdot & \cdot & s_{2L} \\ & & \cdot & & & \cdot \\ & & & & & \\ & & & \cdot & & \cdot \\ & \bigcirc & & & \cdot & \cdot \\ & & & & & s_{LL} \end{bmatrix}.$$

THEOREM (MYSOVSKIH). *The polynomials*

$$F_j(\mathbf{x}) = s_{1j}\varphi_1(\mathbf{x}) + s_{2j}\varphi_2(\mathbf{x}) + \cdots + s_{jj}\varphi_j(\mathbf{x}) \qquad (j = 1, 2, \cdots, L)$$

form an orthonormal system.

Now in the special case $n = 1$, one has $\varphi_j(x) = x^{j-1}$ with $L = N + 1$, and M is just the "Hankel" matrix in the moments. Moreover, we know in this case $F_j(x) = p_{j-1}(x)$, a polynomial of degree $j - 1$, and $\{p_j(x)\}_{j=0}^{N}$ satisfy

$$xp_{j-1}(x) = \beta_{j-1}p_{j-2}(x) + \alpha_j p_{j-1}(x) + \beta_j p_j(x), \qquad j = 1, \cdots, N, \tag{4.2}$$

where $p_{-1}(x) \equiv 0$. Comparing the coefficients of x^j and x^{j-1} on either side of this identity, one gets

$$s_{jj} = \beta_j s_{j+1,j+1}$$

$$s_{j-1,j} = \alpha_j s_{jj} + \beta_j s_{j,j+1}$$

and so

$$\beta_j = \frac{s_{j,j}}{s_{j+1,j+1}}, \qquad \alpha_j = \frac{s_{j-1,j}}{s_{j,j}} - \frac{s_{j,j+1}}{s_{j+1,j+1}}.$$

Further, if

$$R = \begin{bmatrix} r_{11} & r_{12} & \cdot & \cdot & \cdot & r_{1,N+1} \\ & r_{22} & \cdot & \cdot & \cdot & r_{2,N+1} \\ & & \cdot & & & \cdot \\ & & & & & \\ & & & \cdot & & \cdot \\ & \bigcirc & & & \cdot & \cdot \\ & & & & & r_{N+1,N+1} \end{bmatrix}$$

a straightforward computation shows that

$$s_{jj} = \frac{1}{r_{jj}}, \qquad s_{j,j+1} = \frac{-r_{j,j+1}}{r_{j,j}r_{j+1,j+1}}.$$

Thus

$$\alpha_j = \frac{r_{j,j+1}}{r_{j,j}} - \frac{r_{j-1,j}}{r_{j-1,j-1}}, \qquad j = 1, 2, \cdots, N,$$

$$\beta_j = \frac{r_{j+1,j+1}}{r_{j,j}}, \qquad j = 1, 2, \cdots, N - 1, \tag{4.3}$$

with $r_{0,0} = 1$, $r_{0,1} = 0$.

5. Description of Computational Procedures. In the microfiche section of this issue there are three ALGOL 60 procedures for performing the algorithms presented above. We have tried to keep the identifiers as close to the notation of the equations as possible without sacrificing storage or efficiency. The weights and abscissas of the quadrature rule are the result of the procedure GAUSSQUADRULE which must be supplied with the recurrence relation by either procedure GENORTHOPOLY or CLASSICORTHOPOLY. The former requires the moments of the weight function and the latter the name of the particular orthogonal polynomial. A short description of each procedure follows.

CLASSICORTHOPOLY produces μ_0 and the normalized three term recurrence relationship (a_j, b_j) for six well-known kinds of orthogonal polynomials:

KIND = 1, Legendre polynomials $P_n(x)$ on $[-1.0, +1.0]$, $\omega(x) = 1.0$.

KIND = 2, Chebyshev polynomials of the first kind $T_n(x)$ on $[-1.0, +1.0]$, $\omega(x) = (1 - x^2)^{-1/2}$.

KIND = 3, Chebyshev polynomials of the second kind $U_n(x)$ on $[-1.0, +1.0]$, $\omega(x) = (1 - x^2)^{+1/2}$.

KIND = 4, Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$ on $[-1.0, +1.0]$, $\omega(x) = (1 - x)^\alpha(1 + x)^\beta$ for $\alpha > -1$ and $\beta > -1$.

KIND = 5, Laguerre polynomials $L_n^{(\alpha)}(x)$ on $[0, +\infty)$, $\omega(x) = e^{-x}x^\alpha$ for $\alpha > -1$.

KIND = 6, Hermite polynomials $H_n(x)$ on $(-\infty, +\infty)$, $\omega(x) = e^{-x^2}$.

Notice that this procedure requires a real procedure to evaluate the gamma function $\Gamma(x)$.

GENORTHOPOLY uses the 2N + 1 moments of the weight function which are supplied in MU[0] through MU[2 ⊗ N] to compute the α_j's and β_j's of formula (4.2). First, the Cholesky decomposition (formula 4.1) of the moment matrix is placed in the upper right triangular part of the array R, then the formulas (4.3) are used to compute the α_j's and β_j's which are placed in the arrays A and B respectively.

GAUSSQUADRULE has two modes of operation controlled by the Boolean parameter SYMM which indicates whether the tridiagonal matrix is symmetric or not. When the recurrence relation is produced by GENORTHOPOLY or by CLASSICORTHOPOLY, SYMM is *true*. If SYMM is *false*, the matrix is symmetricized using the formulas (2.2). The diagonal elements α_i are stored in A[I] and the off diagonal elements β_i are stored in B[I].

Beginning at label SETUP, several calculations and initializations are done: the l_1 norm of the tridiagonal matrix and the relative zero tolerance are computed; the first component of each eigenvector W[I] and the Q-R iteration are initialized. LAMBDA is a variable subtracted off the diagonal elements to accelerate convergence of the Q-R iteration and control to some extent in what order the eigenvalues (abscissas) are found. It begins with a value (= NORM) outside and to the right of the interval containing the abscissas and moves to the left as the abscissas are found; thus the abscissas will be in ascending order in the array T (just to be sure an exchange sort is used at label SORT).

The maximum (EIGMAX) of the eigenvalues (LAMBD1 and LAMBD2) of the lower 2 × 2 submatrix is compared to the maximum (RHO) from the last iteration. If they are close, LAMBDA is replaced by EIGMAX. This scheme seems to stabilize LAMBDA and speed convergence immediately after deflation.

An eigenvalue has been found when the last off diagonal element falls below EPS (see Section 6). Its value is placed in T[I] and the corresponding weight W[I] is computed from formula (2.5). This convergence test and the test for matrix splitting are done following label INSPECT. Only the lower block (from K to M) needs to be transformed by the *Q-R* equation given in formulas (3.3). These equations have been rearranged to reduce the number of computer operations as suggested by W. Kahan in a report by Corneil [2].

TABLE

A Comparison of the Abscissas and Weights of the Gauss-Laguerre Quadrature Rule with $\alpha = -0.75$ *and* $N = 10$

	Analytic Recurrence Relationship + QR	Moment Matrix + QR	Concus et al [1].
	ABSCISSAS		
1	$2.766655867080153_{10}-2$	$2.766655862878470_{10}-2$	$2.76665586707972_{10}-2$
2	$4.547844226059642_{10}-1$	$4.547844219368714_{10}-1$	$4.54784422605949_{10}-1$
3	$1.3824257611586\underline{19}$	$1.382425759256\underline{314}$	1.382425761158599
4	$2.8339800120927\underline{34}$	$2.8339800085\underline{61162}$	2.833980012092697
5	$4.8509714487649\underline{68}$	$4.850971443\underline{442301}$	4.850971448764914
6	$7.5000109426428\underline{96}$	$7.500010935\underline{563904}$	7.500010942642825
7	$1.0888408023834\underline{46}_{10}+1$	$1.088840801\underline{516104}_{10}+1$	$1.0888408023834404_{10}+1$
8	$1.5199478044237\underline{65}_{10}+1$	$1.519947803\underline{419274}_{10}+1$	$1.519947804423760\underline{3}_{10}+1$
9	$2.0789214621070\underline{18}_{10}+1$	$2.078921460\underline{989977}_{10}+1$	$2.078921462107010\underline{7}_{10}+1$
10	$2.8573060164922\underline{23}_{10}+1$	$2.857306015\underline{294401}_{10}+1$	$2.85730601649221\underline{06}_{10}+1$
	WEIGHTS		
1	$2.56676555779085\underline{3}$	$2.56676555693228\underline{5}$	2.566765557790772
2	$7.7334797034431\underline{68}_{10}-1$	$7.733479706\underline{154000}_{10}-1$	$7.73347970344341_{10}-1$
3	$2.3313283497321\underline{82}_{10}-1$	$2.331328355\underline{3678223}_{10}-1$	$2.33132834973219_{10}-1$
4	$4.6436747089566\underline{77}_{10}-2$	$4.643674724\underline{992909}_{10}-2$	$4.64367470895670_{10}-2$
5	$5.5491235020362\underline{56}_{10}3$	$5.549123531\underline{829512}_{10}-3$	$5.54912350203625_{10}-3$
6	$3.6564666267764\underline{41}_{10}-4$	$3.656466653\underline{186007}_{10}-4$	$3.65646662677638_{10}-4$
7	$1.1868798571025\underline{25}_{10}-5$	$1.186879867\underline{642139}_{10}-5$	$1.18687985710245_{10}-5$
8	$1.5844109420568\underline{44}_{10}-7$	$1.584410958\underline{350144}_{10}-7$	$1.58441094205678_{10}-7$
9	$6.1932667267968\underline{67}_{10}-10$	$6.193266797\underline{518338}_{10}-10$	$6.19326672679684_{10}-10$
10	$3.0377599265176\underline{91}_{10}-13$	$3.037759963\underline{698451}_{10}-13$	$3.03775992651750_{10}-13$

(Underlined figures are those which disagree with Concus et al [1].)

6. Test Program and Results. The procedures in the microfiche section have been extensively tested in Burroughs B5500 Algol and IBM OS/360 Algol. There are two machine dependent items which must be mentioned. First, the constant used to define the "relative zero tolerance" EPS in procedure GAUSSQUADRULE is dependent on the length of the fraction part of the floating-point number representation ($= 8^{-13}$ for the 13 octal digit fraction on the B5500, and $= 16^{-14}$ for a 14 hexadecimal digit long-precision fraction on the IBM 360). Second, the moment matrix M defined in Section 4 usually becomes increasingly ill conditioned with increasing N. Thus the round-off errors generated during Cholesky decomposition in GENORTHOPOLY cause an ill conditioned M to appear no longer positive definite and the procedure fails on taking the square root of a negative number.

The procedure GAUSSQUADRULE proves to be quite stable and when the recursion coefficients are known or supplied by the procedure CLASSICORTHOPOLY it loses only several digits off from full-word accuracy even for $N = 50$. Procedure GENORTHOPOLY usually failed to produce the recursion coefficients from the moments when N was about 20 for the IBM 360.

The driver program given in the microfiche section of this issue is designed to compare the two methods of generating the quadrature rules—from the moments or the recursion coefficients. N can be increased until GENORTHOPOLY fails. Numerical results may be checked against tables for Gauss-Legendre quadrature in [11] and Gauss-Laguerre quadrature in [1]. In the Table, we compare the abscissas and weights of the Gauss-Laguerre quadrature rule with $\alpha = -0.50$ and $N = 10$ computed by: (A) the analytic recurrence relationship and the Q-R algorithm; (B) the moment matrix and the Q-R algorithm; (C) Concus et al. [1]. The calculations for (A) and (B) were performed on the IBM 360.

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