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GENERALIZED KRONROD PATTERSON TYPE IMBEDDED QUADRATURES

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Summary. We present algorithms for the determination of polynomials orthogonal with respect to a positive weight function multiplied by a polynomial with simple roots inside the interval of integration. We apply these algorithms to search for and calculate all possible sequences of imbedded quadratures of maximal polynomial order of precision for the generalized Laguerre and Hermite weight functions.

Keywords: Gaussian quadrature, orthogonal polynomials, Kronrod extensions, Patterson sequences, imbedded quadratures, Laguerre weight function, Hermite weight function

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1. Introduction

In adaptive quadrature algorithms and elsewhere it is often desirable to use sequences of quadrature formulae $\{Q_1(f), Q_2(f), \ldots\}$ which are such that the knots of $Q_i(f)$ are a subset of the knots of $Q_{i+1}(f)$, $i = 1, 2, \ldots$. These sequences of *imbedded* quadratures are usually required to have high polynomial order of precision.

We are thus concerned with sequences $\{Q_i(f)\}_{i=1}^{n}$ of interpolatory quadrature formulae which are such that $Q_1(f)$ has knots $\{v_j^{(1)}\}_{j=1}^{k_1}$ and exact polynomial order of precision $2k_1$, $Q_2(f)$ has knots $\{v_j^{(1)}\}_{j=1}^{k_1} \cup \{v_j^{(2)}\}_{j=1}^{k_2}$ and polynomial order of precision at least $2k_2+k_1$ and in general $Q_n(f)$ has knots $\bigcup_{i=1}^{n} \{v_j^{(i)}\}_{j=1}^{k_i}$ and polynomial order of precision at least $k_n + \sum_{i=1}^{n} k_i$. Consequently $Q_{i+1}(f)$ is determined from $Q_i(f)$ as a Gauss quadrature with prescribed knots.

More precisely, let $w(t)$ be a real valued weight function on some (finite, semi-infinite or infinite) real interval (a, b) such that

$$I(f) := \int_a^b f(t)w(t)\,\mathrm{d}t \tag{1.1}$$

exists for any polynomial $f(t)$. The quadrature formula

$$(1.2) \qquad Q(f) := \sum_{j=1}^{n}\sum_{i=1}^{n_j} C_{ji} f^{(i-1)}(x_j) + \sum_{j=1}^{m}\sum_{i=1}^{m_j} D_{ji} f^{(i-1)}(v_j)$$

using fixed (prescribed) distinct knots $v_1, v_2, \ldots, v_m$ of multiplicities $m_1, m_2, \ldots, m_m$ is said to be Gaussian if the weights (C_{ji} and D_{ji}) and the free (Gauss) knots $x_1, x_2, \ldots, x_n$, of multiplicities $n_1, n_2, \ldots, n_n$ are chosen so that $I(f) = Q(f)$ whenever f is a polynomial of degree $N + n - 1$ or less. Here

$$(1.3) \qquad N := \sum_{j=1}^{n} n_j + \sum_{j=1}^{m} m_j$$

is the number of weights in the quadrature.

Determination of the weights in (1.2) amounts to solving a system of linear algebraic equations while simple Gauss knots are characterized as the zeros of a polynomial orthogonal with respect to the weight function $w(t) \prod_{j=1}^{m} (t - v_j)^{m_j}$. In fact, in this paper we restrict our attention to the case of simple prescribed and Gauss knots v_j and x_j i.e. $n_j = m_j = 1$ (see [2] and the references there for more on quadratures of the type (1.2) without these restrictions).

When simple knots are prescribed inside the interval of integration the existence and the properties of the required quadratures depend on polynomials orthogonal with respect to a weight function which changes sign inside the interval. For some degrees such polynomials may not exist or may have zeros which are multiple, outside (a, b) or even complex. Consequently the resulting quadratures may not exist or may have knots and weights which render them useless.

In [5] Kronrod computed, for the case of the constant weight function, quadratures using $2n + 1$ simple knots of which n are the zeros of the nth degree Legendre polynomial and the other $n + 1$ are Gaussian ($n \leqslant 40$). Patterson [7] later extended these quadratures by adding free knots to quadratures which have the Kronrod knots prescribed. In both [7] and [5] the quadratures were computed by determining the required polynomials from the moments of the weight function and then solving for their roots. Patterson improved Kronrod's method of determining the polynomials by expressing them as linear combinations of Legendre polynomials. Piessens and Branders [8] used Chebyshev rather than Legendre polynomials to further stabilize the process. In [3] Kahaner *et al* investigate, by similar methods, the existence of extended Gauss-Laguerre-Kronrod Quadratures with up to 10 prescribed knots and up to 18 added knots.

One can avoid dealing directly with polynomials by seeking their zeros as the eigenvalues of certain matrices. In [2] Golub and Kautsky show how to compute Gauss Quadratures of the type (1.2) for which the polynomials in question are orthogonal with respect to a non-negative weight function. They use the (symmetric tridiagonal) Jacobi matrix the elements of which are the coefficients in the three-term recurrence satisfied by the orthogonal polynomials. The eigenvalues of the principal submatrices of this matrix are the roots of the polynomials and so they are the knots of the Gaussian quadratures. In [4] we extended the results of [2] to the case where simple prescribed knots in (a, b) cause the weight function to change sign inside the interval of integration. We generalized the concept of Jacobi matrices for non-negative weight functions—when orthogonal polynomials of all degrees exist—to the case where only certain degree polynomials are orthogonal with respect to the required weight function. To replace the Jacobi matrix we introduced there a pair of matrices—the recurrence matrix of the polynomials and the Gram matrix measuring their orthogonality—which we called the Jacobi pair. We also showed the relation between Jacobi pairs for two weight functions related by a linear factor. This led to a numerical method for the calculation of one Jacobi pair from another. In [1] we showed how, given a Jacobi pair for the weight function $w(t)$, it is possible to efficiently compute the Jacobi pair for $r(t)w(t)$, r an arbitrary polynomial. Some simple examples of Kronrod-Patterson quadratures were computed to demonstrate the viability of the method.

In this paper we present sequences of quadratures computed by the above techniques. The sequences we are seeking generalize those of Kronrod and Patterson in two ways. Firstly, we have used the Laguerre and Hermite weight functions and can, in general, use any non-negative weight function w for which we know the Jacobi matrix and $\mu_0 := \int w(t)dt$, the zero-th moment of w. Secondly, we have sought (within the limits of usefulness) all sequences possible and not only those with $k_{i+1} = 1 + \sum_{j=1}^{i} k_j$. We have thus sought quadrature *trees* which we discuss in more detail in §2.

In §3-5 we review the methods and establish some results which lead to the computational procedure given in §6. The tables of results are described and discussed in §7.

2. Quadrature trees

We seek to describe all possible sequences of imbedded Gauss quadratures, for the weight function w, which start with k_1 Gauss knots. Each sequence is a path in a quadrature tree in which a node of depth i represents a quadrature Q_i and all branches from this node represent possible sequences of which Q_i is a non-terminating member.

A sequence can be considered to terminate for any of several reasons. We have already mentioned that for some choices of k_{i+1} there may exist no orthogonal polynomial of appropriate degree and hence no quadrature of the type we seek. If the orthogonal polynomial exists but has complex zeros then the branch will terminate. Of somewhat more interest is the case where some $Q_i(f)$ has knots which are real but lie outside the interval of integration or has negative weights. In some situations quadrature sequences of this type may be useful if only some of the Q_i in the sequence have these undesirable properties.

More precisely, a branch may terminate for the following reasons:

(a) no orthogonal polynomial of the appropriate degree exists,

(b) the orthogonal polynomial has complex zeros,

(c) the orthogonal polynomial has all roots real but some are outside the interval of integration,

(d) all zeros of the orthogonal polynomial are real and inside the interval of integration but some of the weights are negative,

(e) for practical reasons, whenever $k_{i+1} > \max(3k_i, N + k_i/2)$.

Cases (a) and (b) clearly indicate the end of a sequence. In some applications quadratures of the type (c), however, may be useable (ODEs). If the condition described in case (d) occurs in only one quadrature in the sequence then the rest of the sequence may still be useful. Generally, negative weights are a hazard from the point of view of round-off accumulation but if the weights which are negative are relatively small this may not be a problem. In §7, where we list the numerical results, we present estimators which quantify the extent of this hazard.

For $k_{i+1} < k_i + 1$ the branches terminate because condition (a) applies, as we show later. Although we know of no theoretical upper bound on k_{i+1} we have included condition (e) because an imbedded sequence with sharply increasing numbers of knots has little advantage over a sequence of simple Gauss quadratures.

In the next four sections we establish some basic relations, briefly review the method of [1] and describe some implementation details.

3. Modifying a Jacobi pair of matrices

We deal only with functions of a real variable. Let $k > 0$ be an integer and let $\mathbf{p} = (p_1, p_2, \ldots, p_{k-1})^T$ and p_k be a set of polynomials such that $p_j(t)$ has exact degree j. There exists a lower Hessenberg matrix $\mathbf{K}$, with all elements on the super-diagonal non-zero such that

$$t\mathbf{p}(t) = \mathbf{K}\mathbf{p}(t) + \mathbf{e}_k p_k(t)\beta_k, \tag{3.1}$$

β_k a non-zero constant. Here, as later, $\mathbf{e}_k$ is the k-th column of an identity matrix of appropriate dimension. We call $\mathbf{K}$ the recurrence matrix for these polynomials. Since the polynomials are of exact degree they are linearly independent and so $\mathbf{p}(t)$ cannot vanish for any t. Consequently any root v of $p_k(t)$ is an eigenvalue of $\mathbf{K}$. We will denote by $\mathbf{M}$ the symmetric Gram matrix

$$\mathbf{M} := \int_a^b \mathbf{p}\mathbf{p}^T w\mathrm{d}t. \tag{3.2}$$

When the polynomials $p_j(t)$ are orthonormal with respect to $w(t)$, $\mathbf{M}$ is an identity and $\mathbf{K}$ is the (symmetric) Jacobi matrix. We are interested in the case where orthogonal polynomials of all orders may not exist so $\mathbf{M}$ may no longer be diagonal. We say $\mathbf{M}$ is j-diagonal if $\mathbf{M} := [m_{rs}]$ has $m_{rj} = m_{jr} = 0$, $r = 1, 2, \ldots, j-1$. For such an $\mathbf{M}$ we have that $p_{j-1}(t)$ is orthogonal with respect to w and its roots are eigenvalues of the $(j-1) \times (j-1)$ principal submatrix of $\mathbf{K}$.

In [4] and [1] the following results are established.

Theorem 3.1. *Let the exact degree polynomials $p_0, p_1, \ldots, p_k$ have recurrence matrix $\mathbf{K}$ and let the exact degree polynomials $\hat{p}_0, \hat{p}_1, \ldots, \hat{p}_k$ be such that*

$$\mathbf{p} := \mathbf{L}\hat{\mathbf{p}}, \quad p_k = \hat{p}_k + \mathbf{c}^T\hat{\mathbf{p}}, \tag{3.3}$$

where $\mathbf{L}$ is a unit lower triangular matrix and $\mathbf{c}$ is some vector. Then the recurrence matrix $\hat{\mathbf{K}}$ for $\hat{p}_0, \hat{p}_1, \ldots, \hat{p}_k$ satisfies

$$\hat{\mathbf{K}} = \mathbf{L}^{-1}\mathbf{K}\mathbf{L} + \mathbf{e}_k\mathbf{c}^T\beta_k. \tag{3.4}$$

By (3.4) the matrix $\hat{\mathbf{K}} - \mathbf{e}_k\mathbf{c}^T\beta_k$, which differs from $\hat{\mathbf{K}}$ only in its last row, is similar to $\mathbf{K}$ and has the property that, although all its eigenvalues are those of $\mathbf{K}$, the eigenvalues of its principal $j \times j$ submatrix (each $j < k$) are the zeros of $\hat{p}_j(t)$.

Theorem 3.2. *If, in addition to Theorem 3.1, $\hat{w}(t) := r(t)w(t)$ where $r(t)$ is a polynomial of degree m, we define $\mathbf{M}$ as in (3.2) and*

$$\hat{\mathbf{M}} := \int_a^b \hat{\mathbf{p}}\hat{\mathbf{p}}^T\hat{w}dt,$$

then

$$r(\mathbf{K})\mathbf{M} = \mathbf{L}\hat{\mathbf{M}}\mathbf{L}^T + \mathbf{Z}_1 \tag{3.5}$$

where

$$\mathbf{Z}_1 \in \mathcal{Z} := \{\mathbf{Z} \mid \mathbf{e}_j^T\mathbf{Z} = 0^T, \quad j = 1, 2, \ldots, k-m\},$$

i.e. $\mathbf{Z}_1$ is a matrix which vanishes but for its last m rows. Furthermore, if $\mathbf{M}$ and $r(\mathbf{K})$ are non-singular then

$$\hat{\mathbf{K}} = \hat{\mathbf{M}}\mathbf{L}^T\mathbf{M}^{-1}r(\mathbf{K})^{-1}\mathbf{K}\mathbf{L} + \mathbf{Z}_2, \tag{3.6}$$

where $\mathbf{Z}_2 \in \mathcal{Z}$.

In case we start with a Jacobi pair $\mathbf{J}, \mathbf{I}$ which corresponds to orthonormal polynomials then from (3.6) we can compute $\hat{\mathbf{K}}$ from the simpler expression

$$\hat{\mathbf{K}} = \hat{\mathbf{M}}\mathbf{L}^T r(\mathbf{J})^{-1}\mathbf{J}\mathbf{L} + \mathbf{Z}_3, \tag{3.7}$$

where again $\mathbf{Z}_3 \in \mathcal{Z}$.

We remark that the process for modifying a Jacobi pair described here can be viewed as a generalization of the LR process with shifting for the eigenvalues of a matrix. Indeed, for the pair $\mathbf{J}, \mathbf{I}$, the left hand side $r(\mathbf{J})$ of (3.5) is the generalization of the shift $\mathbf{J} - v\mathbf{I}$ and the $\hat{\mathbf{M}}\mathbf{L}^T$ is the R factor. The restoring shift in $\mathbf{RL} + v\mathbf{I}$ becomes the $r(\mathbf{J})^{-1}\mathbf{J}$ factor between the generalized R and L factors on the right hand side of (3.7). While the LR transformation is a similarity, here the $\mathcal{Z}$ matrices cause the assignment of the new eigenvalues.

4. Review of the method

Theorem 3.1 gives in (3.4) the relation between recurrence matrices of any two exact degree polynomial bases. For any $\mathbf{K}, \mathbf{M}$ (representing the polynomial base $\mathbf{p}$ and w) and the polynomial $r(t)$ there are many pairs $\hat{\mathbf{K}}, \hat{\mathbf{M}}$ (representing some other base $\hat{\mathbf{p}}$ and $\hat{w} = rw$). Theorem 3.2 gives a second relation, (3.5), which every such pair must satisfy. Thus starting from a pair $\mathbf{K}, \mathbf{M}$ if we can find any $\mathbf{L}$ and $\hat{\mathbf{M}}$ satisfying (3.5) we can use (3.4) or (3.6) to find $\hat{\mathbf{K}}$, which is uniquely determined by this choice of $\mathbf{L}$ and $\hat{\mathbf{M}}$.

Since we are in search of Gaussian quadratures we want to be sure that as many as possible of the polynomials in the base $\hat{\mathbf{p}}$ to which we transform are orthogonal with respect to the modified weight function, $\hat{w}$. That means that we want to chose an $\hat{\mathbf{M}}$ which is j-diagonal for as many values of j as possible.

In [4], whenever $\hat{\mathbf{M}}$ was not j-diagonal because it was not possible to find a polynomial of degree $j-1$ which was orthogonal to all polynomials of lower degree, the $j-1$ polynomial was chosen either to reduce the sum of squares of off-diagonal elements in $\hat{\mathbf{M}}$ or for convenience. As an improvement we suggest in [1] a scheme which is motivated by the following argument.

If the transformation matrix $\mathbf{L}$ takes one set of polynomials orthonormal with respect to a non-negative weight function into another also orthonormal with respect to a non-negative weight function then both recurrence matrices will be tridiagonal and both Gram matrices will be identities. If in addition the polynomial r is positive on the interval of orthogonality then the left hand side of (3.5) is positive definite and the factoring required in (3.5) can be chosen as a Choleski decomposition. When the left hand side of (3.5) is indefinite but orthonormal polynomials of all degrees exist then an $\mathbf{LDL}^T$ type factoring with $\mathbf{D}$ diagonal but indefinite is possible. But when not all degree orthogonal polynomials exist the Gram matrix $\mathbf{M}$ cannot be diagonal. However, in view of the preceding discussion it seems natural to choose a block $\mathbf{LDL}^T$ type factoring in which the $\mathbf{D}$ matrix is block diagonal and the $\mathbf{L}$ matrix is still unit lower triangular. Any correspondingly chosen polynomial, say of degree s, which is not orthogonal to all polynomials of lower degree will nevertheless be orthogonal to all polynomials of degree $0, 1, \ldots, t < s$ where t is, in a sense, maximized.

In [1] we show that it is possible, given $\mathbf{K}, \mathbf{M}$ and a polynomial r of degree m, to incrementally build up all but the last m columns of a unit lower triangular $\mathbf{L}$ and all but the bottom right $m \times m$ submatrix of the symmetric matrix $\hat{\mathbf{M}}$, both satisfying (3.5), without computing the corresponding $\mathbf{Z}_1$. This is sufficient to uniquely determine all but the last m rows of $\hat{\mathbf{K}}$. We therefore have a way of transforming from one Jacobi pair to another. We form the left hand side of (3.5) of dimension $k := n + m$ and find only those parts of the factors $\mathbf{L}$ and $\hat{\mathbf{M}}$ which are needed in (3.6), or equivalently, to determine a $\hat{\mathbf{K}}$ matrix of dimension n. We discuss the details of this computation in §6 below.

Note that only the bottom right $m \times m$ square of $\mathbf{Z}_1$ in (3.5) is in fact not known because the first $n-m$ columns of the last m rows of $\mathbf{Z}_1$ are known from the symmetry of $\mathbf{L}\hat{\mathbf{M}}\mathbf{L}^T$.

5. Factoring a symmetric indefinite matrix

We are concerned here with factoring the symmetric matrix $\mathbf{A} := r(\mathbf{K})\mathbf{M} - \mathbf{Z}_1 = \mathbf{L}\hat{\mathbf{M}}\mathbf{L}^T$. We construct it in the form

$$\mathbf{A} = \hat{\mathbf{L}}\mathbf{D}\hat{\mathbf{L}}^T \tag{5.1}$$

where $\hat{\mathbf{L}}$ is block lower triangular and $\mathbf{D}$ is diagonal. In fact since $\hat{\mathbf{L}} = \mathbf{LQ}$ with $\mathbf{L}$ lower triangular and $\mathbf{Q}$ block diagonal we get (3.5) with $\hat{\mathbf{M}} = \mathbf{QDQ}^T$.

Since the polynomial $r(t)$ may change sign at the eigenvalues of $\mathbf{K}$ then the matrix being factored may be indefinite and may have vanishing leading principal minors. However the factoring in (3.5) is such that no pivoting may be used and the matrix $\mathbf{L}$ must be lower triangular. In [1] we prove the following.

Theorem 5.1. *Let $\mathbf{A}_i$ denote the order i leading principal submatrix of $\mathbf{A}$, $i = 1, 2, \ldots, k$, and let $0 = s_0 < s_1 < \ldots < s_u = k$ be such that $\mathbf{A}_{s_j}$, $j = 1, 2, \ldots, u-1$ are non-singular. Then there exists a unique decomposition (5.1) with diagonal blocks in $\hat{\mathbf{L}}$ of orders $s_j - s_{j-1}$, $j = 1, 2, \ldots, u$.*

The following algorithm factors a matrix $\mathbf{A}$, such as in Theorem 5.1 above, into the form (5.1) with the special choice $\mathbf{D} := \mathbf{E} := \text{diag}(\pm 1, \pm 1, \ldots, \pm 1)$. The matrix $\hat{\mathbf{L}}$, produced during the factoring, overwrites the block lower triangle of $\mathbf{A}$.

Define the sets of integers $p_i := \{s_i + 1, s_i + 2, \ldots, s_{i+1}\}$ and $q_i := \{s_{i+1}, s_{i+1} + 1, s_{i+1} + 2, \ldots, k\}$. We denote by $\mathbf{A}_{x,y}$ the matrix block consisting of the rows with the indecies in the set x and columns with indecies in the set y.

Algorithm 1:

(a) To start, set $\hat{\mathbf{L}} = \mathbf{O}$, $\mathbf{E} = \mathbf{O}$, both $k \times k$,

(b) for $i = 0, 1, 2, \ldots, u-1$, factor $\mathbf{A}_{p_i,p_i} = \mathbf{Q}_i\mathbf{D}_i^2\mathbf{E}_i\mathbf{Q}_i^T$, $\mathbf{Q}_i$ orthogonal, $\mathbf{D}_i$ diagonal, $\mathbf{E}_i := \text{diag}(\pm 1, \pm 1, \ldots, \pm 1)$ all of dimension $(s_{i+1} - s_i) \times (s_{i+1} - s_i)$,

(c) set $\hat{\mathbf{L}}_{p_i,p_i} = \mathbf{Q}_i|\mathbf{D}_i|$,
(d) set $\mathbf{E}_{p_i,p_i} = \mathbf{E}_i$,
(e) set $\mathbf{Y} = \mathbf{A}_{q_i,p_i}\mathbf{Q}_i|\mathbf{D}_i|^{-1}$,
(f) set $\hat{\mathbf{L}}_{q_i,p_i} = \mathbf{Y}\mathbf{E}_i$,
(g) set $\mathbf{A}_{q_i,q_i} = \mathbf{A}_{q_i,q_i} - \hat{\mathbf{L}}_{q_i,p_i}\mathbf{E}_i\hat{\mathbf{L}}^T_{q_i,p_i}$.

At termination we have all the rows of columns 1 to s_{u-1} of $\hat{\mathbf{L}}$ and $\mathbf{E}$.

This decomposition will have been determined without computing the symmetric eigen-decomposition of a block which includes the unknown $\mathbf{Z}_1$ as long as $s_{u-1} \leqslant k - m$.

6. The practical procedure

Suppose we wish to compute a quadrature (1.2) approximating (1.1) where the $n+m$ order Jacobi pair $\mathbf{J}, \mathbf{I}$ for $w(t)$ is known. We will consider only the case where the prescribed and Gauss knots are all simple; the generalization to multiple knots analogous to that decribed in [2] is possible. We define the $r(t)$ of Theorem 3.2 as

$$r(t) := \prod_{i=1}^{m}(t - v_i).$$

Algorithm 2:

Given $\mathbf{J}$, $r(t)$, n and m,
(a) factor $\mathbf{J} = \mathbf{P}\mathbf{\Lambda}\mathbf{P}^T, \mathbf{P}$ orthogonal, $\mathbf{\Lambda} := \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_{n+m})$,
(b) if $r(\mathbf{\Lambda})$ is singular increase n by 1 and go to step (a),
(c) form $r(\mathbf{J}) = \mathbf{P}r(\mathbf{\Lambda})\mathbf{P}^T$,
(d) use the singular value decomposition to determine s_1, s_2, …, s_u as in Theorem 5.1 with $s_{u-1} \leqslant n$,
(e) factor $\mathbf{A} := r(\mathbf{J}) - \mathbf{Z}_1 = \hat{\mathbf{L}}\mathbf{E}\hat{\mathbf{L}}^T$ by Algorithm 1,
(f) form $\tilde{\mathbf{K}} := \mathbf{E}\hat{\mathbf{L}}\mathbf{P}r(\mathbf{\Lambda})^{-1}\mathbf{\Lambda}\mathbf{P}^T\hat{\mathbf{L}}$,
(g) compute the eigenvalues of each principal submatrix of $\tilde{\mathbf{K}}$ of dimension s_j, $j = 1, 2, \ldots, u-1$.

In step (f) of Algorithm 2, rather than producing $\hat{\mathbf{K}}$, we form a matrix $\tilde{\mathbf{K}}$ which is block diagonally similar to it and thus each of its principal submatrices of order s_j, $j = 1, 2, \ldots, u-1$ has the same eigenvalues as the corresponding submatrix of $\hat{\mathbf{K}}$.

Each such set of eigenvalues is the set of knots for a Gaussian quadrature with the roots of $r(t)$ as prescribed knots.

We must observe that it may not be possible to determine the numbers s_i, in step (d) of Algorithm 2, numerically. However, we can sometimes know *a priori*, from the symmetry of a quadrature or from the fact that a quadrature formula has exact polynomial order of precision higher than the minimum possible, that an orthogonal polynomial of the required degree exists. The next Theorem is relevant here.

Theorem 6.1. *Let $w(t) \geqslant 0$ and the polynomial $r(t)$, of degree m, be such that for some s, $1 \leqslant s \leqslant m$,*

$$\int_a^b t^j r(t)w(t)\mathrm{d}t = \begin{cases} 0 & \text{for } j = 0, 1, 2, \ldots, s-1, \\ \neq 0 & \text{for } j = s. \end{cases} \tag{6.1}$$

Let J be the Jacobi matrix for the polynomials, $p_0(t)$, $p_1(t)$, $p_2(t)$, ..., $p_k(t)$ orthonormal on (a, b) with respect to $w(t)$, $k > s + m$. Then

$$\mathbf{e}_i^T r(\mathbf{J})\mathbf{e}_j = 0 \quad \forall i + j \leqslant s + 1, \tag{6.2}$$

and so the first s principal submatrices of $r(\mathbf{J})$ are singular. If in addition $w(t)$ is symmetric on (a, b) and $r(t)$ is anti-symmetric and of odd degree then using the notation of Theorem 5.1 with $\mathbf{A} := r(\mathbf{J})$ we have
(a) $m + s$ is always even and,
(b) $m + s_j$ is always odd.

Proof. Relation (3.1) for this case is

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

Induction on m shows that

$$r(t)\mathbf{p}(t) = r(\mathbf{J})\mathbf{p}(t) + \mathbf{z}_m \tag{6.3}$$

where $\mathbf{z}_m$ is a degree $k + m - 1$ polynomial vector with $\mathbf{e}_j^T\mathbf{z}_m = 0$, $\forall j \leqslant k - m$. Multiplication of (6.3) on the right by $\mathbf{p}^T(t)w(t)$ and integration on (a, b) gives

$$\int_a^b \mathbf{p}(t)\mathbf{p}^T(t)r(t)w(t)\mathrm{d}t = r(\mathbf{J}) + \mathbf{Z}_4, \tag{6.4}$$

where $\mathbf{Z}_4 \in \mathcal{Z}$, from which (6.2) follows immediately by (6.1). The singularity of the principal submatrices is then obvious.

Now assume that the additional conditions of the theorem hold. Then if $m + s$ is odd the integrand in (6.1) is anti-symmetric when $j = s$ and the integral vanishes. This contradicts the assumption of the Theorem and so $m + s$ must be even. To show that $m + s_j$ is odd when m is odd we note that in general

$$\mathbf{e}_i^T r(\mathbf{J})\mathbf{e}_j \begin{cases} = 0 & \text{when } i + j + m \text{ is odd} \\ \neq 0 & \text{when } i + j + m \text{ is even} \end{cases}$$

Thus for m odd $r(\mathbf{J})$ has a chequerboard pattern of zeros starting with a zero in the (1,1) position. Since any odd dimension matrix with this property is singular the result follows. □

Suppose now that we have determined $\{Q_l(f)\}_{l=1}^{i}$ and we want to know for which values of k_{i+1} there are quadratures $Q_{i+1}(f)$ with the required properties. Recall (Turan [9]) that a necessary and sufficient condition for $Q_i(f)$ to have exact polynomial order of precision $k_i + \sum_{l=1}^{i} k_l$ is that

$$r(t) := \prod_{l=1}^{i} \prod_{j=1}^{k_i} (t - v_j^{(l)}) \tag{6.5}$$

be such that

$$\int_a^b t^j r(t) w(t) \mathrm{d}t = 0, \quad j = 0, 1, 2, \ldots, k_i - 1.$$

Thus we know from Theorem 6.1 that $k_{i+1} > k_i$ and in Step (d) of Algorithm 2 we know that $s_1 > k_i$. This saves k_i singular value decompositions. Furthermore, for the case where $w(t)$ is symmetric, $m := \sum_{l=1}^{i} k_i$ is odd and r(t) is anti-symmetric we know that k_{i+1} must be even and all odd dimensioned principal submatrices of $r(\mathbf{J})$ are known to be singular.

7. Numerical Results

General description.
We present quadrature trees for the generalized Laguerre and Hermite weight functions. These are characterized by

$w(t)$	Interval	Constraints	Name
$t^\alpha e^{-t}$	$[0, \infty]$	$\alpha > -1$	Laguerre
$\lvert t\rvert^\alpha e^{-t^2}$	$[-\infty, \infty]$	$\alpha > -1$	Hermite

We have restricted the computation to the case $\alpha = 0$ only because we are not aware of other useful choices of α. We would welcome the opportunity to compute quadrature trees for other values of α or other $w(t)$ for which the Jacobi matrix and μ_0 are known explicitly and which may be considered to be of special interest or usefulness.

Estimators assessing the weights. We wish here to quantify the extent to which the negative weights of a quadrature formula may adversely affect its usefulness. Let ρ be the sum of absolute values of all the weights. As the first measure we use

$$\sigma_1 := \rho/\mu_0 - 1.$$

Clearly, $\sigma_1 = 0$ indicates that all weights are non-negative and the further σ_1 is from zero the more the quadrature formula may suffer from the accumulation of round off errors when it is being evaluated.

This estimator is sufficient when all weights in the quadrature formula are of the same order. However, quadratures with rapidly decaying weight functions, like the Laguerre and Hermite, have very small weights at the outlying knots. In this case a quadrature formula with small σ_1 may still have relatively large weights at outlying knots. To take account of this we use two further estimators: the first is

$$\sigma_2 := \max_j |\zeta_j|$$

where ζ_j is the ratio between the weight of our quadrature and the weight of the Gauss quadrature, for the same weight function and total number of knots, both at the $j-th$ knot ordered, say, in increasing magnitude. The idea behind this estimator is that it compares our quadrature with the optimal positive-weight quadrature using the same number of knots. This estimator is expensive to compute. The second, cheaper, estimator we use is

$$\sigma_3 := \max_j \frac{N|C_j|}{\mu_o|w(x_j)|}$$

where C_j is the weight corresponding to the knot x_j and N is as in (1.3).

Presentation of the results.

Information concerning the trees we have investigated is laid out in the following way. In each line of a table the column labelled 0 is coded to flag (with a $*$) those nodes of a tree which represent a *good* quadrature formula (those with all knots inside the interval of integration and with positive weights), or those nodes which terminate a branch because we did not pursue it (/). Each quadrature formula the existence or properties of which we are investigating, is represented in column 1 by the numbers of knots added at each stage k_1 k_2 .... The designation $-k_i$ indicates that, although all knots in the sequence are real, some knot(s) in that branch of the sequence fall outside the interval of integration. Column 2 shows the total number of knots that such a quadrature formula would have and in column 3 we show the number $k_n + \sum_{i=1}^{n} k_i$. This number represents a lower bound on the polynomial order of precision that such a formula will have in general. For symmetric measures and an odd number of symmetrically placed knots such a quadrature formula would have polynomial order of precision one higher. Apart from the known cases (e.g. Gegenbauer weight function $(1 - t^2)^\alpha$ for a certain range of α where the Kronrod extension of an n point Gauss formula has polynomial order of precision $4n+2$), there may be instances where the polynomial order of precision of a formula is higher than expected. Columns 4 to 8 contain knot information and columns 9 to 12 contain weights information. Columns 13 and 14 contain the information used to decide whether the orthogonal polynomial of the required degree exists.

More precisely, column 4 shows the number of real zeros of the orthogonal polynomial which lie outside the interval of integration, and column 5 gives a measure d of how far from the interval of integration the most distant knot lies. The integer i in column 5 is coded to mean (ε :=machine epsilon)

d	i
$d \leqslant -0.8$	-9
$-0.8 < d \leqslant -0.7$	-8
$\vdots$	$\vdots$
$-0.1 < d \leqslant -\varepsilon$	-1
$-\varepsilon < d \leqslant \varepsilon$	0
$\varepsilon < d \leqslant 0.1$	1
$\vdots$	$\vdots$
$0.9 < d$	9

Column 6 gives the number of complex zeros of the orthogonal polynomial and column 7 is coded as is column 5 to show the absolute value of the imaginary part of the complex pair which lies furthest from the real line.

Where two knots x_j and x_{N-j+1} lie symmetrically about the origin we use $-\log(x_j + x_{N-j+1})$ to estimate the number of decimal digits to which the computed x_j and x_{N-j+1} agree. The smallest such number for each quadrature formula, which we call the *minimum knot symmetry* is in column 8.

Column 9 displays σ_1 coded in the same way as d and 10 and 11 display the other weights indicators as $\log \sigma_2$ and $\log \sigma_3$ respectively. Column 12 shows the *minimum weight symmetry* computed analogously to the minimum knot symmetry.

Column 13 shows the $2-$ *norm* condition number of the block of $r(\mathbf{J})$ which gave rise to this quadrature formula and column 14 shows $-\log \zeta_k$, ζ_k the smallest singular value of that block.

To illustrate these data Table 1 shows an extract from our complete Gauss-Hermite tree. One can make the following observations:

- There exists a Gauss-Hermite sequence with 1 2 6 10 16 knots. (By definition no Gauss-Hermite quadrature formula knots are outside the interval of integration so columns 4 and 5 of this table contain only zero entries.)
- The 1 2, 1 2 6, and 1 2 6 10 16 quadratures all have non-negative weights but the 1 2 6 10 quadrature formula has some negative weights (in fact these are $-0.011232\ldots$ at $\pm 2.0232\ldots$). The indicator σ_1 lies between ε and 0.1 indicating that no absolutely *large* negative weights exist but $\log \sigma_2 = 3$ shows that at least

one of the weights is about 1000 times as large as the corresponding weight in the Gauss quadrature with the same number of knots.

- Knots of the 1 2 6 10 16 quadrature which are symmetrically placed about the origin agree to at least 28 decimal digits and the weights agree to 27 digits. The knots and weights were computed without taking advantage of symmetry to provide a further check on accuracy.
- No 1 2 4 or 1 2 6 8 Gauss-Hermite quadrature formula exists because the orthogonal polynomials for these quadratures have 2 and 6 complex roots, respectively. The complex pair in the 1 2 4 quadrature formula has imaginary parts that lie between 0.5 and 0.6 units from the real line and the 1 2 6 8 case has a complex pair with imaginary part lying further than 0.9 units from the real line.
- The branches corresponding to quadrature formulae with 1 2 6 10 16 44 through to 1 2 6 10 16 52 knots were not examined because the corresponding blocks of the matrix $r(\mathbf{J})$ had condition numbers which were too large (arbitrarily, we cut off at $\varepsilon^{-2/3}$). This was flagged by the / in column 0.

Table 1 thus contains a portion of a complete search over all the possible extensions we have considered.

As an example, the knots and weights of the 1 2 6 10 16 quadrature formula are displayed in Table 4.

All calculations were performed on a VAX 11/785 with quadruple precision arithmetic (34 decimal digits), repeated in double precision (16 decimal digits) and the two sets of results compared. One can draw various conclusions from the fact that two particular computations of the same number agree to, say, d digits. Very conservatively, one can say that the double precision result is accurate to d digits. Alternatively, assuming that the error of the computaion is independent of the precision used, one can conclude that $\theta := 34 - 16 + d$ digits of the quadruple precision result are correct.

In Tables 2 and 3 we present only those quadratures which have no complex knots. These tables have two additional columns, 15 and 16, which show the minima for the numbers θ representing the accuracy of the knots and the weights respectively.

In a few cases the double precision calculation was not completed because the condition of the relevant blocks was too large. For these cases (marked by a #) a second computation of the quadrature was performed in quad precision but using a blocking different from the first. The entries in these columns show the minimum d for the knots and weights of the quadratures. Two rather special quadratures (marked by ##) have one or two weights ($O(10^{-37})$ and $O(10^{-55})$), which are smaller by many orders of magnitude than all the other weights. The two quad computations for these particular weights agree to 14 and 10 decimals, as explained in the text to the tables, but for all the other weights the computations agree to at least 22 decimals. Otherwise, the imbedded sequences of good quadrature formulae are correct to at least 22 decimal digits. Most, as can be seen from tables 2 and 3 however, are correct to more figures.

In the quadratures of Table 4, d is at least 10 for all knots and weights excepting the two extremely small weights (of order 10^{-18}) for which $d = 8$. We conclude that the knots and weights we have obtained are accurate to at least 26 decimals.

The knots and weights of the good quadrature formulae and the complete trees, from which the information above has been extracted, are readily available from the authors in either hard copy or machine readable form.

Conclusions. Monegato [6] points out that Kronrod extensions with positive weights and real knots do not exist for the Gauss-Laguerre ($\alpha = 0$) weight function while the Gauss-Hermite ($-1 < \alpha \leqslant 1$) extensions can exist only for $n = 1, 2, 4$. Our results seem to indicate that the Hermite 4 5 rule has negative weights for $-1 < \alpha \leqslant +0.39\ldots$ and for $\alpha > 7.6\ldots$.

Even though Kronrod (and hence Patterson) extensions rarely exist for these weight functions our results establish the existence of many useful sequences of imbedded quadratures of maximal polynomial order of precision.

Tables

In the tables below a $*$ indicates that the knots to the quadrature are all real and the weights are non-negative. Column 1 shows the knot sequence, column 2 the total number of points in the quadrature and column 3 its polynomial order of precision. Columns 4–8 give more information about the knots and 9–12 information about the weights. Where shown, column 15 shows the number of decimal digits in the knots which are deduced correct from the double/quad comparisons and column 16 shows the corresponding numbers for the weights. This accuracy test was performed only for the $*$ quadratures. A full explanation of the legend is in the text.

Legend: # – This indicates that no double precision result was available because of the failure of the double precision computation. The figures here show the minimum number of decimal digits which agree between two quad precision calculations of the same quadrature using different blocking choices.

Table 1: Extract from the complete Gauss-Hermite tree

0	1	2	3	4	5	6	7	8	9	10	11	12	13	14
*	1 2	3	5	0	0	0	0	33	0	0	0	33	0	0
	1 2 4	7	11	0	0	2	5	0					1	0
*	1 2 6	9	15	0	0	0	0	32	0	1	1	31	2	0
	1 2 6 8	17	25	0	0	6	9	0					4	0
	1 2 6 10	19	29	0	0	0	0	31	1	3	1	30	5	0
	1 2 6 10 12	31	43	0	0	10	9	0					8	−3
	1 2 6 10 14	33	47	0	0	10	6	0					8	−3
*	1 2 6 10 16	35	51	0	0	0	0	28	0	7	1	27	9	−3
	1 2 6 10 16 18	53	71	0	0	16	9	0					15	−9
	1 2 6 10 16 20	55	75	0	0	16	9	0					15	−9
	1 2 6 10 16 22	57	79	0	0	4	2	0					16	−9
	1 2 6 10 16 24	59	83	0	0	16	5	0					17	−9
	1 2 6 10 16 26	61	87	0	0	10	9	0					18	−9
	1 2 6 10 16 28	63	91	0	0	6	9	0					19	−9
	1 2 6 10 16 30	65	95	0	0	8	9	0					19	−9
	1 2 6 10 16 32	67	99	0	0	10	9	0					20	−9
	1 2 6 10 16 34	69	103	0	0	12	9	0					20	−10
	1 2 6 10 16 36	71	107	0	0	10	9	0					21	−10
	1 2 6 10 16 38	73	111	0	0	16	9	0					21	−10
	1 2 6 10 16 40	75	115	0	0	10	6	0					21	−10
	1 2 6 10 16 42	77	119	0	0	10	7	0					22	−10
/	1 2 6 10 16 44	79	123										23	−9
/	1 2 6 10 16 46	81	127										23	−10
/	1 2 6 10 16 48	83	131										23	−10
/	1 2 6 10 16 50	85	135										23	−10
/	1 2 6 10 16 52	87	139										24	−10
*	1 2 6 10 18	37	55	0	0	0	0	28	0	6	1	25	10	−3
	1 2 6 10 18 20	57	77	0	0	20	9	0					22	−3
	1 2 6 10 18 22	59	81	0	0	20	9	0					18	−9

Table 1: Extract from the complete Gauss-Hermite tree.

Table 2: Gauss-Hermite quadrature sequences.

0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
*	1 2	3	5	0	0	0	0	33	0	0	0	33	0	0	33	32
*	1 2 6	9	15	0	0	0	0	32	0	1	1	31	2	0	31	31
	1 2 6 10	19	29	0	0	0	0	31	1	3	1	30	5	0		
*	1 2 6 10 16	35	51	0	0	0	0	28	0	7	1	27	9	−3	27	24
*	1 2 6 10 18	37	55	0	0	0	0	28	0	6	1	25	10	−3	27	24#
	1 2 6 10 22	41	63	0	0	0	0	26	1	6	2	24	12	−3		
	1 2 6 10 24	43	67	0	0	0	0	26	1	4	9	17	12	−3		
	1 2 6 12	21	33	0	0	0	0	31	3		3		1	29	5	0
*	1 2 6 12 28	49	77	0	0	0	0	27	0	8	1	22	12	−5	25	22#
	1 2 6 12 34	55	89	0	0	0	0	25	1		8	1	19	13	−5	
	1 2 6 12 36	57	93	0	0	0	0	23	1	5	11	10	14	−4		
	1 2 6 14	23	37	0	0	0	0	30	9	3	2	29	5	0		
	1 2 6 14 22	45	67	0	0	0	0	27	9	8	2	22	11	−6		
	1 2 6 14 24	47	71	0	0	0	0	26	9	6	3	18	11	−6		
	1 2 6 14 28	51	79	0	0	0	0	25	7	7	2	19	12	−6		
	1 2 6 14 32	55	87	0	0	0	0	24	7	9	2	18	14	−6		
	1 2 6 14 34	57	91	0	0	0	0	23	7	8	2	17	14	−6		
*	1 2 8	11	19	0	0	0	0	32	0	0	1	30	2	0	32	31
*	1 2 8 20	31	51	0	0	0	0	30	0	3	1	25	7	−1	29	26
*	1 2 8 22	33	55	0	0	0	0	28	0	2	2	22	7	−1	29	22
*	1 4	5	9	0	0	0	0	33	0	0	1	32	0	0	32	32
	1 4 8	13	21	0	0	0	0	32	1	1	1	31	2	0		
*	1 4 8 14	27	41	0	0	0	0	30	0	4	1	28	7	−1	32	29
*	1 4 8 16	29	45	0	0	0	0	30	0	4	1	26	7	−1	30	27
*	1 4 8 18	31	49	0	0	0	0	28	0	4	1	26	8	−1	29	26
*	1 4 10	15	25	0	0	0	0	32	0	1	1	30	3	0	26	31
*	1 4 12	17	29	0	0	0	0	32	0	1	1	30	3	0	29	31
*	1 4 12 34	51	85	0	0	0	0	17	0	6	1	12	11	−4		
*	1 6	7	13	0	0	0	0	33	0	0	1	31	1	0	28	32
*	1 6 12	19	31	0	0	0	0	32	0	2	1	30	4	0	31	31
*	1 6 14	21	35	0	0	0	0	31	0	2	1	29	4	0	29	31
*	1 6 16 23 39	0	0	0	0	30	0	0	2	26	5	0	28	30		
*	2 3	5	8	0	0	0	0	33	0	0	1	33	1	1	33	33
*	2 3 4	9	13	0	0	0	0	32	0	1	1	31	2	1	32	33
	2 3 4 8	17	25	0	0	0	0	31	9	3	1	30	4	0		
	2 3 4 8 24	41	65	0	0	0	0	27	2	6	3	23	10	−3		
*	2 3 4 14	23	37	0	0	0	0	31	0	3	1	28	6	0	30	28

Table 2: Gauss-Hermite quadrature sequences. Continued

0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
*	2 3 6	11	17	0	0	0	0	32	0	1	1	31	2	1	32	31
*	2 3 6 16	27	43	0	0	0	0	30	0	4	1	28	6	−1	31	29
	2 3 6 16 24	51	75	0	0	0	0	25	1	10	2	20	14	−7		
	2 3 6 16 26	53	79	0	0	0	0	25	1	8	2	18	14	−7		
*	2 3 6 18	29	47	0	0	0	0	30	0	3	1	27	6	−1	29	27
*	2 5	7	12	0	0	0	0	33	0	0	1	32	1	1	33	32
*	2 5 14	21	35	0	0	0	0	30	0	2	1	29	4	0	31	29
*	2 7	9	16	0	0	0	0	33	0	0	1	32	2	1	33	31
*	2 7 16	25	41	0	0	0	0	27	0	3	1	27	5	−1	27	26
*	2 7 18	27	45	0	0	0	0	27	0	2	1	25	5	−1	27	25
	4 5	9	14	0	0	0	0	32	8	1	1	32	2	0		
*	4 5 8	17	25	0	0	0	0	31	0	3	1	31	4	0	31	30
	4 5 8 18		35	53	0	0	0	0	28	9	6	2	26	10	−2	
*	4 5 10	19	29	0	0	0	0	31	0	3	1	30	5	0	31	29
	4 5 14	23	37	0	0	0	0	30	9	3	1	29	6	1		
*	4 7	11	18	0	0	0	0	32	0	1	1	32	2	0	32	32
*	4 9	13	22	0	0	0	0	32	0	1	1	30	2	0	32	31
*	4 10	14	24	0	0	0	0	31	0	1	1	31	3	1	31	31
*	4 10 18	32	50	0	0	0	0	29	0	5	1	27	9	−1	29	26
	4 10 19	33	52	0	0	0	0	29	9	5	1	27	9	−1		
*	4 10 20	34	54	0	0	0	0	29	0	3	3	23	9	−1	28	22
*	4 10 21	35	56	0	0	0	0	29	0	5	1	25	10	0	26	22#
*	4 10 23	37	60	0	0	0	0	29	0	3	17	17	10	0	25	22/14##
	4 10 25	39	64	0	0	0	0	29	1	5	1	24	11	0		
*	4 11	15	26	0	0	0	0	32	0	0	1	29	3	1	32	28
	4 11 26	41	67	0	0	0	0	27	9	5	2	23	9	−3		
	4 11 28	43	71	0	0	0	0	27	1	5	1	22	9	−3		
*	6 9	15	24	0	0	0	0	32	0	2	1	31	3	0	32	30
*	6 9 14	29	43	0	0	0	0	31	0	5	1	28	8	−1	30	28
*	6 9 16	31	47	0	0	0	0	29	0	3	10	22	9	−1	28	22
*	6 11	17	28	0	0	0	0	32	0	2	1	31	3	0	32	30
*	6 13	19	32	0	0	0	0	32	0	1	1	29	4	0	32	28
*	6 14	20	34	0	0	0	0	29	0	2	1	29	5	1	29	29
	6 14 35	55	90	0	0	0	0	26	9	8	2	18	14	−3		
*	6 16	22	38	0	0	0	0	30	0	1	1	28	5	1	29	27
	6 16 33	55	88	0	0	0	0	23	5	9	1	18	14	−5		
*	6 17	23	40	0	0	0	0	31	0	2	1	28	5	1	31	28

Table 2: Gauss-Hermite quadrature sequences. Continued

0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
	8 11	19	30	0	0	0	0	30	2	3	1	29	4	0		
	8 11 16	35	51	0	0	0	0	29	1	7	1	26	9	−3		
	8 11 18	37	55	0	0	0	0	28	1	6	1	24	10	−3		
	8 11 28	47	75	0	0	0	0	24	9	6	2	22	13	−3		
*	8 13	21	34	0	0	0	0	31	0	3	1	28	4	−1	31	30
*	8 15	23	38	0	0	0	0	31	0	2	1	27	5	−1	31	28
*	8 16	24	40	0	0	0	0	29	0	3	1	28	6	1	29	29
*	8 17	25	42	0	0	0	0	31	0	1	12	21	6	1	29	28
	8 19	27	46	0	0	0	0	31	1	3	1	27	6	0		
*	8 22	30	52	0	0	0	0	30	0	3	1	27	7	1	29	26
	8 22 39	69	108	0	0	0	0	22	9	12	2	16	18	−8		

Table 2: Summary showing all the Gauss-Hermite quadrature sequences for which knots and weights were computed.

– As for # above but for this quadrature the knots agree to 25 decimal digits and the weights agree to 22 digits except in the case of one pair of weights, with magnitude $O(10^{-37})$, and which agree to 14 decimal digits.

Table 3: Gauss-Laguerre quadrature sequences.

0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
	1 −2	3	5	1	5	0	0		0	1	−1		1	0		
	1 −2 4 7	11	0	0	0	0	0		2	−1	3		0			
	1 −2 4 7	14	21	0	0	0	0		0	5	−1		7	−2		
	1 −2 4 8	15	23	0	0	0	0		0	5	−1		7	−2		
	1 −2 4 10	17	27	0	0	0	0		2	5	−1		7	−3		
	1 −2 4 11	18	29	0	0	0	0		4	3	−1		7	−4		
	1 −2 4 13	20	33	0	0	0	0		3	5	−1		7	−4		
	1 −2 5	8	13	0	0	0	0		0	2	−1		4	0		
	1 −2 6	9	15	0	0	0	0		0	1	−1		4	0		
	1 −2 6 16	25	41	0	0	0	0		0	7	−1		10	−5		
	1 −2 −7	10	17	1	9	0	0		0	3	−1		5	1		
	1 −2 −7 16	26	42	0	0	0	0		2	9	−1		11	−7		

Table 3: Gauss-Laguerre quadrature sequences. Continued

0	1				2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
	1	−2	−7	17	27	44	0	0	0	0		1	8	−1		11	−7		
	1	−2	8		11	19	0	0	0	0		0	2	−1		3	−1		
	1	−2	8	−13	24	37	1	1	0	0		9	8	−1		12	−5		
	1	−2	8	−14	25	39	2	9	0	0		9	9	−1		12	−6		
	1	−2	8	18	29	47	0	0	0	0		1	9	−1		12	−7		
*	1	3			4	7	0	0	0	0		0	1	1		0	0	32	32
	1	3	5		9	14	0	0	0	0		9	4	3		3	−1		
	1	3	5	8	17	25	0	0	0	0		9	7	2		8	−4		
	1	3	5	9	18	27	0	0	0	0		9	6	3		8	−4		
	1	3	5	10	19	29	0	0	0	0		9	4	54		8	−5		
	1	3	5	11	20	31	0	0	0	0		9	7	3		9	−5		
	1	3	5	12	21	33	0	0	0	0		9	5	3		9	−5		
*	1	3	6		10	16	0	0	0	0		0	3	2		4	−1	31	31
*	1	3	7		11	18	0	0	0	0		0	2	2		4	−1	31	29
*	1	3	8		12	20	0	0	0	0		0	1	9		4	−2	29	24
*	1	3	10		14	24	0	0	0	0		0	3	2		4	−2	30	27
*	1	4			5	9	0	0	0	0		0	1	2		1	0	32	32
*	1	4	10		15	25	0	0	0	0		0	4	2		5	−2	27	27
*	1	5			6	11	0	0	0	0		0	0	2		1	0	32	31
	1	5	11		17	28	0	0	0	0		9	5	4		6	−3		
	1	5	−12		18	30	1	1	0	0		6	3	−1		6	−3		
*	1	5	14		20	34	0	0	0	0		0	5	2		6	−4	28	24
	1	5	15		21	36	0	0	0	0		1	5	3		6	−4		
*	1	6			7	13	0	0	0	0		0	0	2		1	−1	32	30
*	1	6	12		19	31	0	0	0	0		0	5	2		9	−2	27	25
	1	6	13		20	33	0	0	0	0		2	3	3		9	−2		
*	1	6	15		22	37	0	0	0	0		0	5	2		8	−3	27	22
*	1	7			8	15	0	0	0	0		0	0	6		2	0	32	25
*	1	7	12		20	32	0	0	0	0		0	4	2		7	−5	26	24
	1	7	−13		21	34	1	9	0	0		0	6	−1		6	−6		
	2	4			6	10	0	0	0	0		9	1	2		2	0		
*	2	4	7		13	20	0	0	0	0		0	4	2		6	−2	30	28
	2	4	8		14	22	0	0	0	0		6	4	2		6	−2		
	2	4	9		15	24	0	0	0	0		6	2	32		6	−2		
	2	4	10		16	26	0	0	0	0		4	4	2		6	−3		
*	2	5			7	12	0	0	0	0		0	1	2		2	0	33	31
	2	5	−10		17	27	1	9	0	0		9	6	−1		7	−3		
	2	5	−10	30	47	77	0	0	0	0		5	14	−1		19	−15		

Table 3: Gauss-Laguerre quadrature sequences. Continued

0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
*	2 6	8	14	0	0	0	0		0	1	2		2	0	32	30
*	2 7	9	16	0	0	0	0		0	0	6		3	1	32	25
	2 −8	10	18	1	9	0	0		1	2	−1		2	−1		
	2 −8 13	23	36	0	0	0	0		5	7	−1		12	−4		
	2 −8 14	24	38	0	0	0	0		3	5	−1		10	−6		
	2 −8 15	25	40	0	0	0	0		9	8	−1		11	−5		
	2 −8 −17	27	44	1	9	0	0		9	8	−1		11	−6		
	2 −8 −18	28	46	1	9	0	0		1	8	−1		11	−7		
*	3 6	9	15	0	0	0	0		0	2	2		3	−1	30	30
*	3 7	10	17	0	0	0	0		0	2	2		3	0	31	29
*	3 8	11	19	0	0	0	0		0	1	2		3	−1	31	26
	3 −9	12	21	1	9	0	0		0	2	−1		4	−1		
	3 −9 −18	30	48	1	9	0	0		9	10	−1		18	−3		
*	4 8	12	20	0	0	0	0		0	3	2		3	−2	30	29
*	4 9	13	22	0	0	0	0		0	1	2		4	−1	30	27
	4 −10	14	24	1	9	0	0		1	3	−1		3	−2		
*	4 11	15	26	0	0	0	0		0	3	2		3	−3	30	27
*	5 9	14	23	0	0	0	0		0	4	2		5	−1	29	28
*	5 10	15	25	0	0	0	0		0	3	2		5	−2	30	26
	5 −11	16	27	1	9	0	0		0	4	−1		7	−1		
*	5 12	17	29	0	0	0	0		0	4	2		5	−3	30	25
*	6 11	17	28	0	0	0	0		0	4	2		7	−2	27	26
*	6 12	18	30	0	0	0	0		0	21	50		6	−3	27	10/25##
	6 13	19	32	0	0	0	0		1	5	2		6	−3		
	6 14	20	34	0	0	0	0		1	4	3		6	−4		
*	7 12	19	31	0	0	0	0		0	5	2		6	−4	26	24
*	7 13	20	33	0	0	0	0		0	3	7		6	−4	26	24
*	7 15	22	37	0	0	0	0		0	5	2		7	−5	26	22
*	8 13	21	34	0	0	0	0		0	6	2		10	−2	24	23#
	8 −14	22	36	1	1	0	0		1	4	−1		10	−2		
	8 15	23	38	0	0	0	0		9	6	2		10	−3		
*	8 16	24	40	0	0	0	0		0	6	2		10	−4	24	21#

Table 3: Summary showing all the Gauss-Laguerre quadrature sequences for which knots and weights were computed.

– As for # above but for this quadrature the knots agree to 27 decimal digits and the weights agree to 25 digits except in the case of one pair of weights, with magnitude $O(10^{-55})$, and which agree to 10 decimal digits.

Table 4

Knots and weights for the 1 2 6 10 16 sequence of Gauss-Hermite quadrature formulae. Sigma 1,2,3 are as in the text.

Computed on VAX 11/785 in quadruple precision.

```
MACHINE EPSILON = 9.630D-35
```

1 2 sequence:

Knots	Weights
$0.000000000000000000000000000000D+00$	$1.181635900603677351532111655 56D+00$
$-1.224744871391589049098642037353D+00$	$2.954089751509193378830279138 90D-01$
$1.224744871391589049098642037353D+00$	$2.954089751509193378830279138 90D-01$

```
POLYNOMIAL ORDER OF PRECISION = 5
SIGMA 1= -1.92592994438723585305597794258 4927D-34
SIGMA 2= 1.000000000000000000000000000000004D+00
SIGMA 3= 2.240844535169032411301027730059634D+00
```

1 2 6 sequence:

Knots	Weights
$0.000000000000000000000000000000D+00$	$4.501470097537818482027092021 18D-01$
$-1.224744871391589049098642037353D+00$	$1.681189289476776719659508453 03D-01$
$1.224744871391589049098642037353D+00$	$1.681189289476776719659508453 03D-01$
$-2.959210779063837722311138500535D+00$	$1.670882630688235214613936899 06D-04$
$-2.023230191100515659208320895180D+00$	$1.417311787397910597141778974 87D-02$
$-5.240335474869576451483839135948D-01$	$4.786942854911414880888991118 69D-01$
$5.240335474869576451483839135948D-01$	$4.786942854911414880888991118 69D-01$
$2.023230191100515659208320895180D+00$	$1.417311787397910597141778974 87D-02$
$2.959210779063837722311138500535D+00$	$1.670882630688235214613936899 06D-04$

```
POLYNOMIAL ORDER OF PRECISION = 15
SIGMA 1= -1.540743955509788682444782354067942D-33
SIGMA 2= 4.218657282483369521514548068185277D+00
SIGMA 3= 5.391370962480835242976052784016956D+00
```

1 2 6 10 sequence:

Knots	Weights
$0.000000000000000000000000000000D+00$	$5.378816070051010398757848640 49D-01$
$-1.224744871391589049098642037353D+00$	$1.136072989574826596263456860 30D-01$
$1.224744871391589049098642037353D+00$	$1.136072989574826596263456860 30D-01$
$-2.959210779063837722311138500535D+00$	$1.065658977285223609738238588 41D-04$
$-2.023230191100515659208320895180D+00$	$-1.123243848906919122254358349 36D-02$

Table 4 Continued

$-5.24033547486957645148383913594 8D-01$	$3.69246433689208725292842090463D-01$
$5.24033547486957645148383913594 8D-01$	$3.69246433689208725292842090463D-01$
$2.02323019110051565920832089518 0D+00$	$-1.12324384890691912225435834936D-02$
$2.95921077906383772231113850053 5D+00$	$1.06565897728522360973823858841D-04$
$-4.49959939831038880288429511940 0D+00$	$1.52957177053223973324134687923D-09$
$-3.66777421594633786003793251745 8D+00$	$1.08027672066247628796313943952D-06$
$-2.26651326205678802746598617543 9D+00$	$5.11331743908837734921475476903D-03$
$-1.83570797517518687377303661427 8D+00$	$3.20552430994458680658156670806D-02$
$-8.70040895352902900134956696281 2D-01$	$1.08388619550030099230015174557D-01$
$8.70040895352902900134956696281 2D-01$	$1.08388619550030099230015174557D-01$
$1.83570797517518687377303661427 8D+00$	$3.20552430994458680658156670806D-02$
$2.26651326205678802746598617543 9D+00$	$5.11331743908837734921475476903D-03$
$3.66777421594633786003793251745 8D+00$	$1.08027672066247628796313943952D-06$
$4.49959939831038880288429511940 0D+00$	$1.52957177053223973324134687923D-09$

```
POLYNOMIAL ORDER OF PRECISION = 29
SIGMA 1= 2.53488991734949434165574418962934 4D-02
SIGMA 2= 1.15326481289667898341536640935484 1D+03
SIGMA 3= 1.01776155240614058511347597949792 5D+01
```

1 2 6 10 16 sequence:

Knots	Weights
$0.00000000000000000000000000000 0D+00$	$9.12626753636618015784618751433D-04$
$-1.22474487139158904909864203735 3D+00$	$8.02455181473911204774905924210D-02$
$1.22474487139158904909864203735 3D+00$	$8.02455181473911204774905924205D-02$
$-2.95921077906383772231113850053 5D+00$	$6.33286208056174798926698340755D-05$
$-2.02323019110051565920832089518 0D+00$	$4.09675277203441034424345187364D-03$
$-5.24033547486957645148383913594 8D-01$	$2.62448714887843068475168131330D-01$
$5.24033547486957645148383913594 8D-01$	$2.62448714887843068475168131330D-01$
$2.02323019110051565920832089518 0D+00$	$4.09675277203441034424345187314D-03$
$2.95921077906383772231113850053 5D+00$	$6.33286208056174798926698340746D-05$
$-4.49959939831038880288429511940 0D+00$	$8.15537218169173874335697571146D-10$
$-3.66777421594633786003793251745 8D+00$	$4.37378180409268808882839681361D-07$
$-2.26651326205678802746598617543 9D+00$	$1.45155804251558622875835195102D-03$
$-1.83570797517518687377303661427 8D+00$	$5.59288289114694100849109490240D-03$
$-8.70040895352902900134956696281 2D-01$	$1.63712215557357978737966786231D-01$
$8.70040895352902900134956696281 2D-01$	$1.63712215557357978737966786231D-01$
$1.83570797517518687377303661427 8D+00$	$5.59288289114694100849109490349D-03$
$2.26651326205678802746598617543 9D+00$	$1.45155804251558622875835195116D-03$
$3.66777421594633786003793251745 8D+00$	$4.37378180409268808882839681374D-07$
$4.49959939831038880288429511940 0D+00$	$8.15537218169173874335697571136D-10$

Table 4 Continued

$-6.375939270982235951712703750732D+00$	$1.868401489450941274380347729 80D-18$
$-5.643257857885745062803754283040D+00$	$9.659946627856107403678905718 74D-15$
$-5.036089944473093968685964322632D+00$	$5.489683694849976367020249873 25D-12$
$-4.029220140504371364793504978119D+00$	$3.792022239231961517589995113 07D-08$
$-3.349163953713194977367385026776D+00$	$4.846279973702036001194349429 05D-06$
$-2.570558376584296709113064004430D+00$	$4.878539930444381905440961985 68D-04$
$-1.579412134846767085720367583019D+00$	$2.778050890853509986250619591 26D-02$
$-1.760641420820089350297456865320D-01$	$3.398859558558523765326516122 90D-01$
$1.760641420820089350297456865320D-01$	$3.398859558558523765326516122 90D-01$
$1.579412134846767085720367583011D+00$	$2.778050890853509986250619591 22D-02$
$2.570558376584296709113064004439D+00$	$4.878539930444381905440961985 35D-04$
$3.349163953713194977367385026772D+00$	$4.846279973702036001194349429 14D-06$
$4.029220140504371364793504978124D+00$	$3.792022239231961517589995112 91D-08$
$5.036089944473093968685964322627D+00$	$5.489683694849976367020249873 50D-12$
$5.643257857885745062803754283034D+00$	$9.659946627856107403678905719 67D-15$
$6.375939270982235951712703750730D+00$	$1.868401489450941274380347728 91D-18$

```
POLYNOMIAL ORDER OF PRECISION = 51
SIGMA 1= -1.637040452729150475097581251197188D-33
SIGMA 2= 6.569363395543873950747533272909761D+06
SIGMA 3= 1.667876375457536234427505250556718D+01
```

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