

On the Construction of Gaussian Quadrature Rules from Modified Moments*

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Abstract. Given a weight function $\omega(x)$ on (α, β) , and a system of polynomials $\{p_k(x)\}_{k=0}^{\infty}$, with degree $p_k(x) = k$, we consider the problem of constructing Gaussian quadrature rules $\int_{\alpha}^{\beta} f(x)\omega(x)dx \doteq \sum_{r=1}^n \lambda_r^{(n)} f(\xi_r^{(n)})$ from "modified moments" $v_k = \int_{\alpha}^{\beta} p_k(x)\omega(x)dx$. Classical procedures take $p_k(x) = x^k$, but suffer from progressive ill-conditioning as n increases. A more recent procedure, due to Sack and Donovan, takes for $\{p_k(x)\}$ a system of (classical) orthogonal polynomials. The problem is then remarkably well-conditioned, at least for finite intervals $[\alpha, \beta]$. In support of this observation, we obtain upper bounds for the respective asymptotic condition number. In special cases, these bounds grow like a fixed power of n . We also derive an algorithm for solving the problem considered, which generalizes one due to Golub and Welsch. Finally, some numerical examples are presented.

1. Introduction. Let $\omega(x)$ be a weight function on the (finite or infinite) interval (α, β) , i.e., measurable and nonnegative on (α, β) , with all moments

$$(1.1) \quad \mu_k = \int_{\alpha}^{\beta} x^k \omega(x) dx, \quad k = 0, 1, 2, \dots,$$

finite and $\mu_0 > 0$. Given a set $\{p_k(x)\}_{k=0}^{\infty}$ of polynomials, with degree $p_k = k$, we call

$$(1.2) \quad v_k = \int_{\alpha}^{\beta} p_k(x)\omega(x) dx, \quad k = 0, 1, 2, \dots$$

the *modified moments* of ω . Clearly, $v_k = \mu_k$, if $p_k(x) = x^k$.

A *Gaussian quadrature rule* associated with the weight function ω is a functional

$$(1.3) \quad G_n f = \sum_{r=1}^n \lambda_r^{(n)} f(\xi_r^{(n)}),$$

which has the property that

$$(1.4) \quad G_n f = \int_{\alpha}^{\beta} f(x)\omega(x) dx, \quad \text{all } f \in \mathbf{P}_{2n-1},$$

where \mathbf{P}_{2n-1} is the class of polynomials of degree $\leq 2n - 1$. As is well known, G_n exists uniquely for each $n = 1, 2, 3, \dots$. In fact, the abscissas $\xi_r^{(n)}$ are the zeros of $\pi_n(x)$,

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$$(1.5) \quad \pi_n(\xi_r^{(n)}) = 0, \quad r = 1, 2, \dots, n,$$

where $\{\pi_k(x)\}_{k=0}^\infty$ is the system of orthonormal polynomials belonging to the weight function ω ,

$$(1.6) \quad \text{degree } \pi_k = k, \quad \int_\alpha^\beta \pi_r(x)\pi_s(x)\omega(x) dx = \begin{matrix} = 0 & r \neq s, \\ = 1 & r = s. \end{matrix}$$

The weights $\lambda_r^{(n)}$, too, can be expressed in terms of these polynomials, e.g., by

$$(1.7) \quad \lambda_r^{(n)} = \left(\sum_{k=0}^{n-1} [\pi_k(\xi_r^{(n)})]^2 \right)^{-1}, \quad r = 1, 2, \dots, n,$$

showing that $\lambda_r^{(n)} > 0$.

The problem we want to consider is the computation of the functional G_n (i.e., the computation of the abscissas $\xi_r^{(n)}$ and weights $\lambda_r^{(n)}$), given the modified moments v_k . In view of (1.5), (1.7), the problem may be considered as solved, once the orthonormal polynomials $\{\pi_k\}$ have been obtained accurately.

We note, incidentally, that these polynomials are also useful for the construction of rules

$$(1.3) \sim \quad \tilde{G}_n f = \tilde{\lambda}_1^{(n)} f(\xi) + \sum_{r=2}^n \tilde{\lambda}_r^{(n)} f(\xi_r^{(n)}),$$

where ξ is an arbitrary real number with $\pi_{n-1}(\xi) \neq 0$, and

$$(1.4) \sim \quad \tilde{G}_n f = \int_\alpha^\beta f(x)\omega(x) dx, \quad \text{all } f \in \mathbf{P}_{2n-2}.$$

The abscissas $\xi_r^{(n)}$, $r \geq 2$, are then in fact the zeros (other than ξ) of

$$(1.5) \sim \quad \psi_n(x) = \pi_{n-1}(\xi)\pi_n(x) - \pi_n(\xi)\pi_{n-1}(x),$$

while the weights $\tilde{\lambda}_r^{(n)}$, $r = 1, 2, \dots, n$, are still given by the expression on the right of (1.7), if $\xi_r^{(n)}$ is replaced by $\tilde{\xi}_r^{(n)}$ and $\tilde{\xi}_1^{(n)} = \xi$ [2, Sections I.3–4].

The problem stated, in the special case $p_k(x) = x^k$, is classical, and a number of methods are known for its solution. However, the problem becomes increasingly ill-conditioned as n increases, as we have shown in [6]. In order to obtain high-order Gaussian quadrature rules in this manner, it is therefore necessary to resort to multiple-precision computations. Alternatively, more elaborate procedures may be used, such as the one in [6], which do not rely on the moments μ_k .

The general problem was considered recently by Sack and Donovan [12], in the case of polynomials $\{p_k\}$ satisfying a recurrence relation

$$(1.8) \quad xp_j(x) = a_j p_{j+1}(x) + b_j p_j(x) + c_j p_{j-1}(x), \quad j = 0, 1, 2, \dots; \quad p_{-1}(x) = 0,$$

with known coefficients $a_j \neq 0$, b_j , c_j . If $\{p_k\}$ are themselves orthogonal polynomials (e.g., Legendre polynomials, or Chebyshev polynomials of the first and second kind), and (α, β) is a finite interval, the results reported in [12] suggest that the problem is now remarkably well-conditioned. This new approach is therefore a useful alternative to the procedures mentioned above, in cases where the modified moments are accurately computable.

It seems worthwhile, therefore, to investigate the condition of the general problem in the case of polynomials $\{p_k\}$ which are orthogonal with respect to some other weight function $w(x)$ on the interval (a, b) [not necessarily equal to (α, β)],

$$(1.9) \quad \text{degree } p_k = k, \quad \int_a^b p_r(x)p_s(x)w(x) dx = 0 \quad (r \neq s).$$

Such polynomials always satisfy a recurrence relation of the form (1.8). In Section 2 we obtain upper bounds for the condition number of this problem, relative to both finite and infinite intervals (a, b) . Asymptotic estimates of the condition number are given in Section 3 for certain classical weight functions on the interval $[-1, 1]$. Rather strikingly, these estimates grow only like a fixed power of n . The condition is less favorable, in general, if the interval (α, β) is infinite. In Section 4 we then derive an algorithm for solving the problem under study. The algorithm reduces to one given by Golub and Welsch [8] for the case $p_k(x) = x^k$ and is similar (although not identical) to the algorithm of Sack and Donovan [12]. Some numerical examples are presented in Section 5. In particular, we obtain Gaussian quadrature rules G_n for $n = 1(1)8, 16, 32$, relative to the weight functions

$$\omega(x) = \frac{1}{2} \left(1 + \frac{\cos m\pi x}{\sin m\pi x} \right), \quad m = 1(1)12,$$

on $[-1, 1]$. Tables of the respective Gaussian abscissas and weights may be found on the microfiche card attached to this issue.

2. Condition of the Problem. In studying the condition of our problem, it is convenient to consider normalized modified moments as defined by

$$(2.1) \quad \tilde{v}_k = h_k^{-1/2} \int_a^b p_k(x)\omega(x) dx, \quad k = 0, 1, 2, \dots,$$

where

$$(2.2) \quad h_k = \int_a^b p_k^2(x)w(x) dx.$$

The normalized moments \tilde{v}_k are invariant under different normalizations of the orthogonal polynomials $\{p_k\}$.

The problem stated in Section 1 is then equivalent to solving the system of $2n$ (nonlinear) algebraic equations

$$(2.3) \quad h_k^{-1/2} \sum_{r=1}^n \lambda_r p_k(\xi_r) = \tilde{v}_k, \quad k = 0, 1, 2, \dots, 2n - 1,$$

for the unknowns λ_r, ξ_r . We can write these equations in vector form,

$$(2.4) \quad F(y) = \tilde{v},$$

by letting $y^T = [\lambda_1, \dots, \lambda_n, \xi_1, \dots, \xi_n]$, $\tilde{v}^T = [\tilde{v}_0, \tilde{v}_1, \dots, \tilde{v}_{2n-1}]$, $F^T = [F_0, F_1, \dots, F_{2n-1}]$, and

$$(2.5) \quad F_k(y) = h_k^{-1/2} \sum_{r=1}^n \lambda_r p_k(\xi_r), \quad k = 0, 1, \dots, 2n - 1.$$

In conformity with (1.3), we denote the solution of (2.4) by

$$(2.6) \quad y_0^T = [\lambda_1^{(n)}, \dots, \lambda_n^{(n)}, \xi_1^{(n)}, \dots, \xi_n^{(n)}].$$

Given a vector norm $\|\cdot\|$, and an associated matrix norm, we may define, as in [6], a (relative) asymptotic condition number κ_n for the problem (2.4), viz.

$$(2.7) \quad \kappa_n = \frac{\|\tilde{v}\|}{\|y_0\|} \|[F_y(y_0)]^{-1}\|,$$

where $F_y(y)$ denotes the Jacobian matrix of $F(y)$. An elementary computation shows that

$$(2.8) \quad F_y(y_0) = H \Xi \Lambda,$$

where

$$(2.9) \quad H = \text{diag}(h_0^{-1/2}, h_1^{-1/2}, \dots, h_{2n-1}^{-1/2}), \quad \Lambda = \text{diag}(1, \dots, 1, \lambda_1, \dots, \lambda_n)$$

are diagonal matrices, and

$$(2.10) \quad \Xi = \begin{bmatrix} p_0(\xi_1) \cdots p_0(\xi_n) & p'_0(\xi_1) \cdots p'_0(\xi_n) \\ p_1(\xi_1) \cdots p_1(\xi_n) & p'_1(\xi_1) \cdots p'_1(\xi_n) \\ \dots & \dots \\ p_{2n-1}(\xi_1) \cdots p_{2n-1}(\xi_n) & p'_{2n-1}(\xi_1) \cdots p'_{2n-1}(\xi_n) \end{bmatrix}.$$

(For simplicity, we have written ξ_r for $\xi_r^{(n)}$, and λ_r for $\lambda_r^{(n)}$ in (2.9), (2.10).) Therefore,

$$(2.11) \quad \kappa_n \leq \frac{\|\tilde{v}\|}{\|y_0\|} \|\Lambda^{-1}\| \|\Xi^{-1}H^{-1}\|.$$

For the following, it turns out to be convenient to work with the L_1 -norm

$$(2.12) \quad \|y\|_1 = \sum_{k=0}^{2n-1} |y_k|, \quad y^T = [y_0, y_1, \dots, y_{2n-1}].$$

THEOREM 2.1. *Let $[a, b]$ be a finite interval. With $\{l_\lambda(x)\}_{\lambda=1}^n$ denoting the Lagrange interpolation polynomials associated with the abscissas $\{\xi_r^{(n)}\}_{r=1}^n$,*

$$(2.13) \quad l_\lambda(x) = \prod_{v=1, v \neq \lambda}^n \frac{x - \xi_v^{(n)}}{\xi_\lambda^{(n)} - \xi_v^{(n)}} = \frac{\pi_n(x)}{\pi'_n(\xi_\lambda^{(n)})(x - \xi_\lambda^{(n)})},$$

let

$$(2.14) \quad L_n = \int_a^b \sum_{\lambda=1}^n l_\lambda^2(x) w(x) dx,$$

$$(2.15) \quad \sigma_n = \max_{1 \leq \lambda \leq n} |l'_\lambda(\xi_\lambda^{(n)})|.$$

Let, furthermore,

$$(2.16) \quad M_\mu = \max_{a \leq x \leq b} |p_\mu(x)|, \quad h_\mu = \int_a^b p_\mu^2(x) w(x) dx,$$

$$(2.17) \quad \Delta_n = \max\{|\xi_\lambda^{(n)} - x| : a \leq x \leq b, \lambda = 1, 2, \dots, n\}.$$

Then, using the L_1 -norm (2.12) in (2.7), we have

$$(2.18) \quad \kappa_n \leq \kappa_n^{(1)} \kappa_n^{(2)} \kappa_n^{(3)},$$

where

$$(2.19^1) \quad \kappa_n^{(1)} = \max(1, 1/\min \lambda_r^{(n)}) [1 + (2\sigma_n + 1) \Delta_n] / \left(\mu_0 + \sum_{r=1}^n |\zeta_r^{(n)}| \right),$$

$$(2.19^2) \quad \kappa_n^{(2)} = \max_{0 \leq \mu \leq 2n-1} (M_\mu / h_\mu^{1/2}),$$

$$(2.19^3) \quad \kappa_n^{(3)} = L_n \|\tilde{v}\|_1.$$

Remarks. 1. The quantity $\kappa_n^{(1)}$ depends only on the weight function $\omega(x)$, the quantity $\kappa_n^{(2)}$ only on $w(x)$, while $\kappa_n^{(3)}$ depends on both $\omega(x)$ and $w(x)$.

2. Normally, $[\alpha, \beta] = [a, b]$, in which case $\Delta_n \leq b - a$.

Proof of Theorem 2.1. The key issue in the proof is a bound on the norm of $\Xi^{-1} H^{-1}$. We first determine Ξ^{-1} explicitly.

Let

$$(2.20) \quad P_\lambda(x) = l_\lambda^2(x) [1 - 2l'_\lambda(\zeta_\lambda^{(n)})(x - \zeta_\lambda^{(n)})],$$

$$(2.21) \quad Q_\lambda(x) = l_\lambda^2(x)(x - \zeta_\lambda^{(n)})$$

denote the fundamental Hermite interpolation polynomials belonging to the abscissas $\{\zeta_r^{(n)}\}$. Let

$$(2.22) \quad P_\lambda(x) = \sum_{\mu=0}^{2n-1} a_{\lambda\mu} p_\mu(x), \quad Q_\lambda(x) = \sum_{\mu=0}^{2n-1} b_{\lambda\mu} p_\mu(x).$$

Then, as in [4], one shows that

$$(2.23) \quad \Xi^{-1} = \begin{bmatrix} A \\ B \end{bmatrix}, \quad A = [a_{\lambda\mu}], \quad B = [b_{\lambda\mu}].$$

By the orthogonality of $\{p_\mu(x)\}$, one obtains from (2.22)

$$a_{\lambda\mu} = \frac{1}{h_\mu} \int_a^b P_\lambda(x) p_\mu(x) w(x) dx, \quad b_{\lambda\mu} = \frac{1}{h_\mu} \int_a^b Q_\lambda(x) p_\mu(x) w(x) dx,$$

or, in view of (2.20), (2.21),

$$(2.24) \quad a_{\lambda\mu} = \frac{1}{h_\mu} (\alpha_{\lambda\mu} - 2s_\lambda^{(n)} \beta_{\lambda\mu}), \quad b_{\lambda\mu} = \frac{1}{h_\mu} \beta_{\lambda\mu},$$

where

$$(2.25) \quad s_\lambda^{(n)} = l'_\lambda(\zeta_\lambda^{(n)}),$$

and

$$(2.26) \quad \alpha_{\lambda\mu} = \int_a^b l_\lambda^2(x) p_\mu(x) w(x) dx, \quad \beta_{\lambda\mu} = \int_a^b l_\lambda^2(x) p_\mu(x) (x - \zeta_\lambda^{(n)}) w(x) dx.$$

We are now in a position to bound the norm of $\Xi^{-1} H^{-1}$. From (2.26), we have

$$(2.27) \quad \sum_{\lambda=1}^n |\alpha_{\lambda\mu}| \leq \sum_{\lambda=1}^n \int_a^b l_\lambda^2(x) |p_\mu(x)| w(x) dx \leq M_\mu L_n,$$

$$(2.28) \quad \sum_{\lambda=1}^n |\beta_{\lambda\mu}| \leq \sum_{\lambda=1}^n \int_a^b l_\lambda^2(x) |p_\mu(x)| |x - \xi_\lambda^{(n)}| w(x) dx \leq M_\mu \Delta_n L_n.$$

Therefore, by (2.24),

$$\sum_{\lambda=1}^n |a_{\lambda\mu}| \leq \frac{M_\mu}{h_\mu} (1 + 2 \Delta_n \sigma_n) L_n, \quad \sum_{\lambda=1}^n |b_{\lambda\mu}| \leq \frac{M_\mu}{h_\mu} \Delta_n L_n.$$

Consequently,

$$(2.29) \quad \|\Xi^{-1} H^{-1}\|_1 \leq [1 + (2\sigma_n + 1) \Delta_n] L_n \max_{0 \leq \mu \leq 2n-1} M_\mu / h_\mu^{1/2}.$$

The theorem now follows from (2.11) and (2.29), by observing that

$$(2.30) \quad \|y_0\|_1 = \sum_{r=1}^n (\lambda_r^{(n)} + |\xi_r^{(n)}|) = \mu_0 + \sum_{r=1}^n |\xi_r^{(n)}|,$$

and

$$(2.31) \quad \|\Lambda^{-1}\|_1 = \max(1, 1/\min \lambda_r^{(n)}).$$

The following theorem is not restricted to finite intervals $[a, b]$.

THEOREM 2.2. *Let (a, b) be a finite or infinite interval. In addition to the notations of Theorem 2.1, let*

$$(2.32) \quad \begin{aligned} L_{n,1} &= \int_a^b \left[\sum_{\lambda=1}^n l_\lambda^2(x) \right]^2 w(x) dx, \\ L_{n,2} &= \int_a^b \left[\sum_{\lambda=1}^n l_\lambda^2(x) |x - \xi_\lambda^{(n)}| \right]^2 w(x) dx. \end{aligned}$$

Then, using the L_1 -norm (2.12) in (2.7), we have

$$(2.33) \quad k_n \leq k_n^{(1)} k_n^{(2)},$$

where

$$(2.34) \quad k_n^{(1)} = \frac{\max(1, 1/\min \lambda_r^{(n)})}{\mu_0 + \sum_{r=1}^n |\xi_r^{(n)}|},$$

$$(2.35) \quad k_n^{(2)} = (L_{n,1}^{1/2} + (1 + 2\sigma_n) L_{n,2}^{1/2}) \|\tilde{v}\|_1.$$

Proof. The proof is virtually the same as that for Theorem 2.1, except that the sums in (2.27), (2.28) are estimated differently, using Schwarz's inequality:

$$\begin{aligned} \sum_{\lambda=1}^n |\alpha_{\lambda\mu}| &\leq \int_a^b \sum_{\lambda=1}^n l_\lambda^2(x) |p_\mu(x)| w(x) dx \\ &\leq \left\{ \int_a^b \left[\sum_{\lambda=1}^n l_\lambda^2(x) \right]^2 w(x) dx \int_a^b p_\mu^2(x) w(x) dx \right\}^{1/2} = h_\mu^{1/2} L_{n,1}^{1/2}, \end{aligned}$$

$$\begin{aligned} \sum_{\lambda=1}^n |\beta_{\lambda\mu}| &\leq \int_a^b \sum_{\lambda=1}^n l_\lambda^2(x) |x - \xi_\lambda^{(n)}| |p_\mu(x)| w(x) dx \\ &\leq \left\{ \int_a^b \left[\sum_{\lambda=1}^n l_\lambda^2(x) |x - \xi_\lambda^{(n)}| \right]^2 w(x) dx \int_a^b p_\mu^2(x) w(x) dx \right\}^{1/2} = h_\mu^{1/2} L_{n,2}^{1/2}. \end{aligned}$$

Hence, as previously,

$$\|\Xi^{-1}H^{-1}\|_1 \leq L_{n,1}^{1/2} + (1 + 2\sigma_n)L_{n,2}^{1/2},$$

and Theorem 2.2 follows from (2.11), (2.30), and (2.31).

For infinite intervals (α, β) the bounds in (2.18) and (2.33) are likely to be very large, even for only moderately large n , on account of the smallness of $\min \lambda_r^{(n)}$. Severe ill-conditioning, in such cases, is therefore a potential hazard. Example (iii) of Section 5 illustrates this point.

3. Asymptotic Estimates of Condition Number. We illustrate Theorem 2.1 of the previous section by considering some special (classical) weight functions. We use the notation

$$a_n \sim b_n \text{ as } n \rightarrow \infty$$

to express the fact that $|a_n/b_n|$ remains between positive bounds not depending on n , as $n \rightarrow \infty$.

THEOREM 3.1. *Let $[a, b] = [\alpha, \beta] = [-1, 1]$.*

(a) *If $\omega(x) = (1 - x^2)^\alpha$, $-\frac{1}{2} \leq \alpha \leq 0$, then $\kappa_n^{(1)} \leq \bar{\kappa}_n^{(1)}$, where $\bar{\kappa}_n^{(1)} \sim n^{2\alpha+3}$ as $n \rightarrow \infty$.*

(b) *If $w(x) = (1 - x)^q(1 + x)^\beta$, $\alpha > -1$, $\beta > -1$, then, as $n \rightarrow \infty$, $\kappa_n^{(2)} \sim n^{q+1/2}$ if $q \geq -\frac{1}{2}$, and $\kappa_n^{(2)} \sim 1$ if $q < -\frac{1}{2}$, where $q = \max(\alpha, \beta)$.*

(c) *If $\omega(x) = w(x)$, then $\kappa_n^{(3)} = \mu_0^{3/2}$.*

(d) *If $\omega(x) = (1 - x^2)^\alpha$, $-1 < \alpha \leq 0$, and $w(x) = (1 - x^2)^\beta$, $\beta \geq -\frac{1}{2}$, then $\kappa_n^{(3)} \leq \bar{\kappa}_n^{(3)}$, where, as $n \rightarrow \infty$, $\bar{\kappa}_n^{(3)} \sim n^{\beta+3/2}$ if $\alpha \neq 0$, and $\bar{\kappa}_n^{(3)} \sim n^{\beta+7/2}$ if $\alpha = 0$.***

Proof. (a) The polynomials $\pi_k(x)$, in this case, are the ultraspherical polynomials $P_k^{(\alpha,\alpha)}(x)$, properly normalized. We assume the zeros $\xi_r = \xi_r^{(n)}$ of $P_n^{(\alpha,\alpha)}(x)$ numbered in decreasing order,

$$(3.1) \quad 1 > \xi_1 > \xi_2 > \dots > \xi_n > -1.$$

They are symmetrically distributed with respect to the origin, i.e., $\xi_r = -\xi_{n+1-r}$. It is known [14, p. 121] that for $|\alpha| \leq \frac{1}{2}$,

$$(3.2) \quad \cos\left(r \frac{\pi}{n+1}\right) \leq \xi_r \leq \cos\left(r - \frac{1}{2}\right) \frac{\pi}{n}, \quad r = 1, 2, \dots, [n/2].$$

From this one obtains by an elementary computation

$$\cot \frac{\pi}{2(n+1)} - 1 \leq \sum_{r=1}^n |\xi_r| \leq \frac{1}{\sin(\pi/2n)}.$$

It follows that $\sum_{r=1}^n |\xi_r| \sim n$, and therefore

The result in the case $\alpha = 0$ could be sharpened to read $\bar{\kappa}_n^{(3)} \sim n^{\beta+5/2} \ln^2 n$. See footnote *.

$$(3.3) \quad \mu_0 + \sum_{r=1}^n |\xi_r| \sim n \quad \text{as } n \rightarrow \infty.$$

For the corresponding Christoffel numbers $\lambda_r^{(n)}$ we have [14, p. 350] $\min \lambda_r^{(n)} = \lambda_1^{(n)}$, whenever $\alpha \geq -\frac{1}{2}$. (Note that for $\alpha = -\frac{1}{2}$ all $\lambda_r^{(n)}$ are equal to π/n .) Moreover [14, p. 350], $\lambda_1^{(n)} \sim n^{-2\alpha-2}$. Therefore,

$$(3.4) \quad \max(1, 1/\min \lambda_r^{(n)}) \sim n^{2\alpha+2} \quad \text{as } n \rightarrow \infty.$$

In order to estimate σ_n in (2.15), we recall (see, e.g., [11, p. 63]) that for $\alpha \leq 0$,

$$(3.5) \quad v_\lambda(x) > |\alpha| \quad \text{on } -1 \leq x \leq 1,$$

where

$$v_\lambda(x) = 1 - 2l'_\lambda(\xi_\lambda)(x - \xi_\lambda).$$

We distinguish two cases, depending on whether $l'_\lambda(\xi_\lambda) \geq 0$ or $l'_\lambda(\xi_\lambda) < 0$. In the first case we let $x = 1$ in (3.5), and obtain

$$|l'_\lambda(\xi_\lambda)| < \frac{1 - |\alpha|}{2(1 - \xi_\lambda)}.$$

Using (3.1) and (3.2), we get

$$|l'_\lambda(\xi_\lambda)| < \frac{1 - |\alpha|}{2(1 - \xi_1)} \leq \frac{1 - |\alpha|}{2(1 - \cos(\pi/2n))} = \frac{1 - |\alpha|}{4 \sin^2(\pi/4n)}.$$

In the second case we let $x = -1$ in (3.5) and obtain by a similar reasoning

$$|l'_\lambda(\xi_\lambda)| < \frac{1 - |\alpha|}{2(1 + \xi_\lambda)} \leq \frac{1 - |\alpha|}{2(1 + \xi_n)} \leq \frac{1 - |\alpha|}{4 \sin^2(\pi/4n)}.$$

Thus, in either case,

$$|l'_\lambda(\xi_\lambda)| < \frac{1 - |\alpha|}{4 \sin^2(\pi/4n)},$$

and it follows that

$$(3.6) \quad \sigma_n = \max_\lambda |l'_\lambda(\xi_\lambda)| \leq \bar{\sigma}_n, \quad \bar{\sigma}_n \sim n^2 \quad \text{as } n \rightarrow \infty.$$

Combining (3.3), (3.4), and (3.6) gives the desired result.

(b) With $p_\mu(x) = P_\mu^{(\alpha, \beta)}(x)$, and $q = \max(\alpha, \beta)$, we have for the quantity M_μ in (2.16) [14, p. 166]

$$(3.7) \quad M_\mu = \frac{\Gamma(\mu + q + 1)}{\Gamma(q + 1)\Gamma(\mu + 1)} \sim \mu^q \quad \text{if } q \geq -\frac{1}{2},$$

and

$$(3.8) \quad M_\mu \sim \mu^{-1/2} \quad \text{if } q < -\frac{1}{2}.$$

Since

$$(3.9) \quad h_\mu^{1/2} = 2^{(\alpha+\beta+1)/2} \left[\frac{\Gamma(\mu + \alpha + 1)\Gamma(\mu + \beta + 1)}{(2\mu + \alpha + \beta + 1)\Gamma(\mu + 1)\Gamma(\mu + \alpha + \beta + 1)} \right]^{1/2} \sim \mu^{-1/2},$$

$\mu \rightarrow \infty,$

the assertion follows.

(c) Since $\omega(x) = w(x)$, we have $L_n = \mu_0$ (see, e.g., [11, p. 52]), and $\tilde{v}_0 = \sqrt{\mu_0}$, $\tilde{v}_k = 0$ for $k > 0$, giving $\kappa_n^{(3)} = \mu_0^{3/2}$ as asserted.

(d) In the ultraspherical case $\omega(x) = (1 - x^2)^\alpha$, $-1 < \alpha \leq 0$, it is known that [14, Problems 58, 60]

$$\sum_{\lambda=1}^n I_\lambda^2(x) \leq \frac{1}{|\alpha|} \quad (-1 < \alpha < 0), \quad \sum_{\lambda=1}^n I_\lambda^2(x) \leq \frac{1}{\tan^2(3\pi/4(2n + 1))} \quad (\alpha = 0),$$

uniformly on $[-1, 1]$. Therefore,

$$(3.10) \quad L_n \leq \bar{L}_n, \quad \bar{L}_n = m_0/|\alpha| \quad (-1 < \alpha < 0),$$

$$\bar{L}_n = m_0/\tan^2 \frac{3\pi}{4(2n + 1)} \quad (\alpha = 0),$$

where $m_0 = \int_{-1}^1 w(x) dx$. In particular***,

$$(3.11) \quad \bar{L}_n \sim 1 \quad (-1 < \alpha < 0),$$

$$\bar{L}_n \sim n^2 \quad (\alpha = 0).$$

From (3.7), (3.9) (with $\alpha = \beta = q$) one finds by a simple computation that $M_k/h_k^{1/2}$ is an increasing function of k , if $\beta > -\frac{1}{2}$, and constant (for $k > 0$) equal to $2/\sqrt{\pi}$, if $\beta = -\frac{1}{2}$. Therefore,

$$\|\tilde{v}\|_1 = \sum_{k=0}^{2n-1} |\tilde{v}_k| \leq \mu_0 \sum_{k=0}^{2n-1} M_k/h_k^{1/2} \leq \mu_0 2n M_{2n-1}/h_{2n-1}^{1/2},$$

and using the asymptotic estimates in (3.7) and (3.9),

$$(3.12) \quad \|\tilde{v}\|_1 \leq N_n, \quad N_n \sim n^{\beta+3/2}.$$

The desired result now follows from (3.10)–(3.12). Theorem 3.1 is proved.

As an example, suppose we generate the Gaussian rule G_n associated with the ultraspherical weight function $(1 - x^2)^\alpha$, $-\frac{1}{2} \leq \alpha \leq 0$, using as $\{p_k\}$ the ultraspherical polynomials with parameter β , $-\frac{1}{2} \leq \beta \leq 0$. Then Theorem 3.1, together with (2.18), tells us that the associated condition number κ_n satisfies $\kappa_n \leq \bar{\kappa}_n$, where, as $n \rightarrow \infty$,

$$\bar{\kappa}_n \sim n^{2(\alpha+\beta)+5} \quad \text{if } \alpha \neq 0 \text{ and } \alpha \neq \beta,$$

$$\bar{\kappa}_n \sim n^{2\beta+7} \quad \text{if } \alpha = 0 \text{ and } \beta \neq 0,$$

$$\bar{\kappa}_n \sim n^{3\alpha+7/2} \quad \text{if } \alpha = \beta.$$

***In the case $\alpha = 0$, the sharper estimate $L_n \leq L_n^*$, $L_n^* \sim n \ln^2 n$ could be obtained by using an estimate for $\sum_{\lambda=1}^n |I_\lambda(x)|$, due to G. I. Natanson [10], in conjunction with the inequality $\sum_{\lambda=1}^n I_\lambda^2(x) \leq (\sum_{\lambda=1}^n |I_\lambda(x)|)^2$.

Theorem 3.1, and the example just given, are presented here for the sole purpose of illustrating the magnitude of the condition number for the problem considered. It is not suggested that for such classical weight functions Gaussian quadrature rules be constructed from modified moments, since the respective orthogonal polynomials are explicitly known.

In practice, $\omega(x)$ being given, we have no control over $\kappa_n^{(1)}$. However, we may influence the magnitude of $\kappa_n^{(2)}$, and to some extent that of $\kappa_n^{(3)}$, by an appropriate choice of the polynomials $\{p_k\}$. In this connection, part (b) of Theorem 3.1 suggests the Chebyshev polynomials of the first kind, $p_k(x) = T_k(x)$, as both convenient and well-conditioned. With this choice, in fact, $\kappa_n^{(2)} = (2/\pi)^{1/2}$.

4. An Algorithm for Generating Orthonormal Polynomials. We now derive an algorithm for generating the orthonormal polynomials $\{\pi_k(x)\}_{k=0}^n$ of (1.6), given a set of polynomials $\{p_k(x)\}$ (orthogonal or not), satisfying the recurrence relation

$$(4.1) \quad xp_j(x) = a_j p_{j+1}(x) + b_j p_j(x) + c_j p_{j-1}(x), \quad j = 0, 1, 2, \dots; \\ p_{-1}(x) = 0, \quad a_j \neq 0,$$

and given the associated modified moments $\{v_k\}_{k=0}^{2n}$ of (1.2). Our aim is toward determining the coefficients α_j, β_j ($j = 0, 1, 2, \dots, n - 1$) in the recurrence relation

$$(4.2) \quad x\pi_j(x) = \alpha_j \pi_{j+1}(x) + \beta_j \pi_j(x) + \alpha_{j-1} \pi_{j-1}(x), \quad j = 0, 1, 2, \dots; \quad \pi_{-1}(x) = 0.$$

We denote by

$$(f, g) = \int_a^b f(x)g(x)\omega(x) dx$$

the inner product with respect to which the $\pi_k(x)$ are orthonormal. Let $M = [m_{ij}]$ be the Gram matrix of order $n + 1$, i.e.,

$$(4.3) \quad m_{ij} = (p_i, p_j) \quad (i, j = 0, 1, \dots, n).$$

Clearly, M is positive-definite. Let

$$(4.4) \quad M = R^T R, \quad R = [r_{ij}]$$

be the Cholesky decomposition of M , and

$$(4.5) \quad S = R^{-1}, \quad S = [s_{ij}].$$

Both R and S are upper triangular matrices with positive diagonal elements. By an observation of Mysovskih [9],

$$(4.6) \quad \pi_j(x) = s_{0j} p_0(x) + s_{1j} p_1(x) + \dots + s_{jj} p_j(x), \quad j = 0, 1, \dots, n.$$

Substituting (4.6) into (4.2), we can write

$$x[s_{0j} p_0 + \dots + s_{j-1,j} p_{j-1} + s_{jj} p_j] \\ = \alpha_j [s_{0,j+1} p_0 + \dots + s_{j,j+1} p_j + s_{j+1,j+1} p_{j+1}] + \beta_j [s_{0j} p_0 + \dots + s_{jj} p_j] \\ + \alpha_{j-1} [s_{0,j-1} p_0 + \dots + s_{j-1,j-1} p_{j-1}].$$

Each term on the left, in view of (4.1), can be expressed as a linear combination of p 's. Having done this, coefficients of equal p 's must agree on both sides, because of the linear independence of the system $\{p_k(x)\}$. In particular, comparing the coefficients of p_{j+1} and p_j , one gets

$$s_{jj}a_j = \alpha_j s_{j+1,j+1}, \quad s_{jj}b_j + s_{j-1,j}a_{j-1} = \alpha_j s_{j,j+1} + \beta_j s_{jj},$$

from which

$$\alpha_j = \frac{s_{jj}}{s_{j+1,j+1}} a_j, \quad \beta_j = b_j - \frac{s_{j,j+1}}{s_{j+1,j+1}} a_j + \frac{s_{j-1,j}}{s_{jj}} a_{j-1}.$$

Since

$$s_{jj} = \frac{1}{r_{jj}} \quad (j = 0, 1, \dots, n),$$

$$s_{j,j+1} = -\frac{r_{j,j+1}}{r_{jj}r_{j+1,j+1}} \quad (j = 0, 1, \dots, n - 1),$$

one finally obtains

$$(4.7) \quad \alpha_j = \frac{r_{j+1,j+1}}{r_{jj}} a_j, \quad j = 0, 1, \dots, n - 1.$$

$$\beta_j = b_j + \frac{r_{j,j+1}}{r_{jj}} a_j - \frac{r_{j-1,j}}{r_{j-1,j-1}} a_{j-1},$$

For $j = 0$, $r_{-1,0}$ is to be interpreted as zero, and $r_{-1,-1}$ as an arbitrary nonzero number.

We note that the formulas (4.7) reduce to those of Golub and Welsch [8], if $a_j = 1$, $b_j = c_j = 0$, i.e., $p_k(x) = x^k$. Also, of course, $M = R = I$, and thus $\alpha_j = a_j$, $\beta_j = b_j$, if $p_k(x) = \pi_k(x)$.

Once the Gram matrix M is known, the desired coefficients α_j, β_j can thus be obtained from (4.7) by a Cholesky decomposition of M .

The Gram matrix M , on the other hand, can be built up from the modified moments v_j in the following manner. Applying the recursion (4.1) twice, one has

$$\begin{aligned} m_{ij} &= (p_i, p_j) = \left(\frac{1}{a_{i-1}} [(x - b_{i-1})p_{i-1} - c_{i-1}p_{i-2}], p_j \right) \\ &= \frac{1}{a_{i-1}} [(xp_{i-1}, p_j) - b_{i-1}(p_{i-1}, p_j) - c_{i-1}(p_{i-2}, p_j)] \\ &= \frac{1}{a_{i-1}} [(p_{i-1}, xp_j) - b_{i-1}(p_{i-1}, p_j) - c_{i-1}(p_{i-2}, p_j)] \\ &= \frac{1}{a_{i-1}} [a_j(p_{i-1}, p_{j+1}) + b_j(p_{i-1}, p_j) + c_j(p_{i-1}, p_{j-1}) - b_{i-1}(p_{i-1}, p_j) \\ &\quad - c_{i-1}(p_{i-2}, p_j)], \end{aligned}$$

that is,

$$(4.8) \quad m_{ij} = \frac{1}{a_{i-1}} [a_j m_{i-1,j+1} + (b_j - b_{i-1}) m_{i-1,j} + c_j m_{i-1,j-1} - c_{i-1} m_{i-2,j}].$$

Since

$$(4.9) \quad m_{-1,j} = 0, \quad m_{0j} = p_0 v_j \quad (j = 0, 1, \dots, 2n),$$

we have in (4.8) a recursive scheme to progressively build up the matrix M , using (4.9) as initial values.

The involvement of v_{2n} in (4.9) may appear puzzling at first, the Gaussian rule G_n being determined uniquely by the first $2n$ modified moments $v_j, j = 0, 1, 2, \dots, 2n - 1$. Actually, the role of v_{2n} is just that of normalizing $\pi_n(x)$, and its value affects neither $\xi_r^{(n)}$ nor $\lambda_r^{(n)}$, in view of (1.5), (1.7).

The algorithm presented here does not compare favorably with the algorithm of Sack and Donovan [12] in terms of speed and storage requirements. Our derivation, however, appears to us more transparent than the derivation given in [12].

5. Numerical Examples. All computations described in this section were carried out on the CDC 6500 computer in single precision arithmetic.

(i) We repeat and extend some of the experiments reported by Sack and Donovan [12]. For $p_k(x)$ we choose in turn $x^k, (1 + x)^k, P_k(x), T_k(x), U_k(x)$, where P_k, T_k, U_k denote, respectively, the Legendre polynomial, the Chebyshev polynomials of the first and second kind. We apply the algorithm of Section 4 to produce the coefficients $\alpha_r, \beta_r, r = 0, 1, \dots, n - 1$, in the recurrence relation for the normalized Legendre and Chebyshev polynomials, making use of the appropriate modified moments shown in Table 1. (Notations: $(2n)!! = 2 \cdot 4 \cdots (2n), (2n + 1)!! = 1 \cdot 3 \cdot 5 \cdots (2n + 1), 0!! = (-1)!! = 1, (-3)!! = -1$.)

TABLE 1. Modified moments v_k .

$\omega(x)$		1	$(1 - x^2)^{-1/2}$	$(1 - x^2)^{1/2}$
$p_k(x)$				
x^k	k even	$2/(k+1)$	$(k-1)!!\pi/k!!$	$(k-1)!!\pi/(k+2)!!$
	k odd	0	0	0
	$(1+x)^k$	$2^{k+1}/(k+1)$	$2^k(2k-1)!!\pi/(2k)!!$	$(2k+1)!!\pi/(k+2)!$
$P_k(x)$	k even		$(k!)^2\pi/(k!!)^4$	$-(k-1)!!(k-3)!!\pi/(k!!(k+2)!!)$
	k odd		0	0
$T_k(x)$	k even	$-2/((k+1)(k-1))$		$\pi/2 \quad (k=0)$ $-\pi/4 \quad (k=2)$
	k odd	0		0 (otherwise)
$U_k(x)$	k even	$2/(k+1)$	π	
	k odd	0	0	

For the first two choices of $p_k(x)$, as is to be expected, the Gram matrix M becomes increasingly ill-conditioned with n increasing, and the Cholesky decomposition of M eventually breaks down on taking the square root of a negative number. Prior to this, the errors in α_r and β_r steadily increase, except for β_r in the first case [$p_k(x) = x^k$], where the algorithm consistently returns the correct value $\beta_r = 0$. Sample values of

errors are shown in Table 2 for the case $\omega(x) = 1$. The Cholesky decomposition, in this case, fails at $n = 23$ and $n = 12$, respectively. The situation is very similar for the other two weight functions.

TABLE 2. Errors in the recursion coefficients for normalized Legendre polynomials.

	$p_k(x) = x^k$	$p_k(x) = (1 + x)^k$	
	error in α_r	error in α_r	error in β_r
$r = 5$	1.9×10^{-12}	1.8×10^{-8}	1.1×10^{-8}
10	5.3×10^{-9}	2.3×10^{-2}	1.0×10^{-1}
15	1.9×10^{-5}	—	—
20	2.5×10^{-2}	—	—
25	—	—	—

No problems of any kind are encountered for the remaining three choices of $p_k(x)$, even going with n as high as 100. The coefficients α_r, β_r are obtained essentially to machine accuracy, the largest error observed being 7.1×10^{-14} .

(ii) Weight functions of interest in Fourier analysis are $\omega(x) = c_m(x)$, and $\omega(x) = s_m(x)$, where

$$(5.1) \quad \begin{aligned} c_m(x) &= \frac{1}{2}(1 + \cos m\pi x), \\ s_m(x) &= \frac{1}{2}(1 + \sin m\pi x), \end{aligned} \quad -1 \leq x \leq 1; \quad m = 0, 1, 2, \dots$$

Writing Fourier coefficients in the form [15]

$$(5.2) \quad \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x) \cos mx \, dx = \int_{-1}^1 f(\pi x) c_m(x) \, dx - \int_{-1}^1 f(\pi x) s_0(x) \, dx,$$

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} f(x) \sin mx \, dx = \int_{-1}^1 f(\pi x) s_m(x) \, dx - \int_{-1}^1 f(\pi x) s_0(x) \, dx,$$

$$m = 1, 2, 3, \dots,$$

the first integrals on the right may be calculated by an appropriately weighted Gaussian quadrature rule, and the second integrals by classical Gaussian quadrature. To the best of our knowledge, no extensive tables exist for Gaussian rules G_n associated with the weight functions (5.1). Admittedly, their usefulness is somewhat limited, because the set of points at which f must be evaluated differs from one Fourier coefficient to another.

Our algorithm of Section 4 may be used to generate the required orthonormal polynomials. It is convenient to use it with $p_k(x) = P_k(x)$, since the modified moments can then be expressed in terms of spherical Bessel functions. In fact, using [1, p. 122]

$$\int_{-1}^1 e^{im\pi x} P_k(x) dx = i^k \left(\frac{2}{m}\right)^{1/2} J_{k+1/2}(m\pi),$$

we obtain in the cosine-case

$$(5.3) \quad v_0 = 1, \quad v_{2k} = \frac{(-1)^k}{(2m)^{1/2}} J_{2k+1/2}(m\pi) \quad (k > 0), \quad v_{2k+1} = 0 \quad (k \geq 0),$$

and in the sine-case

$$(5.4) \quad v_0 = 1, \quad v_{2k-1} = \frac{(-1)^{k+1}}{(2m)^{1/2}} J_{2k-1/2}(m\pi) \quad (k > 0), \quad v_{2k} = 0 \quad (k > 0).$$

To compute the Bessel functions in (5.3), (5.4), we use the procedure *Japlus*† of [5], and the Gaussian abscissas and weights have been obtained using the relevant portions (both sequential and nonsequential) of Algorithm 331 [7]. The results are checked by having the quadrature rules regenerate the modified moments.

Table 3 of the microfiche section gives 12D values of $\zeta_r^{(n)}, \pi \zeta_r^{(n)}, \lambda_r^{(n)}$ for the Gaussian rule (1.3) associated with $\omega(x) = c_m(x)$, for $n = 1(1)8, 16, 32, m = 1(1)12$. (Because of symmetry, only the nonnegative abscissas and corresponding weights are listed.) Table 4 contains the analogous information for $\omega(x) = s_m(x), m = 0(1)12$.

(iii) To give an example for an infinite interval, we consider the “one-sided” Gauss-Hermite quadrature rules (1.3) corresponding to $\omega(x) = e^{-x^2}$ on $[0, \infty)$. Tables for such rules were recently published in [13], [3]. It seems natural, in this case, to choose $p_k(x) = H_k(x)$, the Hermite polynomials orthogonal with respect to $\omega(x)$ on $(-\infty, \infty)$. Then clearly,

$$(5.5) \quad v_0 = \sqrt{\pi}/2, \quad v_{2k} = 0 \quad (k > 0).$$

To compute v_{2k+1} , we start from the explicit representation

$$H_{2k+1}(x) = \sum_{r=0}^k (-1)^r \binom{2k+1}{2r} \frac{(2r)!}{2^r r!} 2^{2k+1-r} x^{2k+1-2r}.$$

Multiplying both sides by e^{-x^2} , and integrating between 0 and ∞ , we obtain, in view of $\int_0^\infty e^{-x^2} x^{2k+1-2r} dx = \frac{1}{2}(k-r)!$,

$$v_{2k+1} = \int_0^\infty e^{-x^2} H_{2k+1}(x) dx = \sum_{r=0}^k (-1)^r \binom{2k+1}{2r} \frac{(2r)!}{2^r r!} 2^{2k-r} (k-r)!,$$

or, after simplification,

$$(5.6) \quad v_{2k+1} = \sum_{r=0}^k s_r^{(k)}, \quad s_r^{(k)} = 2^k (-1)^r \prod_{i=r+1}^k (2i) \prod_{i=k-r+1}^k (2i+1).$$

Each $s_r^{(k)}$ being an integer, the sum in (5.6) can be evaluated in integer arithmetic without loss of accuracy, as long as no overflow occurs. Even so, however, it is found that the Gauss abscissas and weights obtained by our algorithm gradually deteriorate

† This procedure calls the gamma function $\Gamma(1+a)$. Since $a = 1/2$ in our application, we have replaced “gamma(1+a)” by its numerical value $\sqrt{\pi}/2 = .88622692545276$ in the procedure body.

in accuracy. For $n = 6$, for example, only 9–11 correct significant digits are obtained, while for $n = 12$ only the first 2–4 significant digits are correct. It is believed that this deterioration of accuracy is a reflection of the progressive ill-conditioning of our problem. The quantity $\min \lambda_r^{(n)}$, in fact, is about 9.8×10^{-5} for $n = 6$, and 1.2×10^{-10} for $n = 12$, resulting in a value of $k_n^{(1)}$ in (2.34) of the order 10^4 and 10^{10} , respectively.

Note Added in Proof. A substantially greater loss of accuracy is observed in Example (iii) if for $p_k(x)$ one chooses the Laguerre polynomials $L_k(x)$ instead of the Hermite polynomials $H_k(x)$. It is found that the Cholesky decomposition (4.4), in this case, breaks down for $n = 7$, and the final results for $n = 6$ are correct to only 3 decimal digits (using single precision arithmetic on the CDC 6500).

It is instructive to compare the condition number κ_n for these two choices of the polynomials $p_k(x)$ on the basis of Theorem 2.2. The constant $k_n^{(1)}$ in (2.34) being the same for both choices of p_k , it suffices to compare $k_n^{(2)}$ in (2.35). Using the Gauss abscissas published in [3] to compute the Lagrange polynomials $l_\lambda(x)$, the quantities $L_{n,1}$ and $L_{n,2}$ in (2.32) may be evaluated by $2n$ -point Hermite quadrature (if $p_k = H_k$) and by $2n$ -point Gauss-Laguerre quadrature (if $p_k = L_k$). This will give $L_{n,1}$ exactly (apart from rounding errors), and $L_{n,2}$ at least approximately. For $n = 6$, one obtains

$$L_{n,1} = 3.25 \times 10^{10}, \quad L_{n,2} = 3.80 \times 10^{11} \quad (p_k = H_k),$$

$$L_{n,1} = 1.72 \times 10^{19}, \quad L_{n,2} = 8.42 \times 10^{21} \quad (p_k = L_k).$$

Since $\|\tilde{v}\|_1$ is of comparable magnitude in both cases (approximately .808 for $p_k = H_k$, and 1.84 for $p_k = L_k$), one concludes that $k_n^{(2)}$ has the order of magnitude 10^6 in the case of Hermite polynomials, but the order of magnitude 10^{11} in the case of Laguerre polynomials.

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