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On Computing Gauss-Kronrod Quadrature Formulae*

By Franca Caliò, Walter Gautschi, and Elena Marchetti

Abstract. We discuss the use of Newton's method for computing Gauss-Kronrod quadrature formulae from modified moments. The underlying nonlinear maps are analyzed from the point of view of numerical condition. A method is indicated of computing the polynomial whose zeros are the Kronrod nodes. Examples include Gauss-Kronrod formulae for integrals with a logarithmic and algebraic singularity at one endpoint. Pertinent numerical results are tabulated in the supplements section at the end of this issue.

1. Introduction. Given a positive measure $d\sigma(t)$ on the real line, whose support contains infinitely many points and all of whose moments exist, we call

$$\int_{\mathbf{R}} f(t)d\sigma(t) = \sum_{\nu=1}^{n} \sigma_\nu f(\tau_\nu) + \sum_{\mu=1}^{n+1} \sigma_\mu^* f(\tau_\mu^*) + R_n(f) \tag{1.1}$$

a *Gauss-Kronrod quadrature formula* if $\tau_\nu = \tau_\nu^{(n)}$ are the Gaussian nodes associated with $d\sigma$ and the nodes τ_μ^* and weights σ_ν, σ_μ^* are chosen so as to maximize the degree of exactness of (1.1). Since there are $3n + 2$ unknowns, we can achieve degree of exactness $d = 3n + 1$, i.e., $R_n(f) = 0$ whenever $f = \mathbf{P}_{3n+1}$. It is well known, in fact, that the nodes τ_μ^* must be the zeros of π_{n+1}^*, the (monic) polynomial of degree $n + 1$ satisfying the orthogonality property

$$\int_{\mathbf{R}} \pi_{n+1}^*(t)\pi_n(t)t^i d\sigma(t) = 0, \qquad i = 0, 1, \ldots, n, \tag{1.2}$$

where $\pi_n(\cdot) = \pi_n(\cdot; d\sigma)$ is the nth degree orthogonal polynomial belonging to the measure $d\sigma$. Note that the measure $d\sigma^*(t) = \pi_n(t; d\sigma)d\sigma(t)$, with respect to which π_{n+1}^* is orthogonal, changes sign. We cannot expect, therefore, that π_{n+1}^* has all its zeros necessarily real.

We are interested here only in Gauss-Kronrod formulae (1.1) with *real* nodes τ_μ^*, all contained in $[a, b]$—the smallest interval containing the support of $d\sigma$—and with *positive* weights σ_μ^*. Then the interlacing property holds (Monegato [17, Theorem 1]),

$$a \leqslant \tau_{n+1}^* < \tau_n < \tau_n^* < \tau_{n-1} < \cdots < \tau_1 < \tau_1^* \leqslant b. \tag{1.3}$$

Our concern is with the actual computation of these nodes and the corresponding weights (provided they exist), given the integer $n \geqslant 1$ and the positive measure $d\sigma$.

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Constructive methods for this problem have been considered before. For the Legendre measure $d\sigma(t) = dt$ on $[-1, 1]$, Kronrod [16] in his original work obtains π_{n+1}^* in power form by solving (1.2). Patterson [22] expands π_{n+1}^* in Legendre polynomials, while Piessens and Branders [23] use Chebyshev polynomials, the nodes τ_μ^* each time being computed by an appropriate rootfinding procedure. The weights can be obtained by interpolation. Monegato [17], [19], Baratella [1], and Dagnino and Fiorentino [3] use similar procedures to compute π_{n+1}^* for Gegenbauer measures and other classical measures. Kahaner et al. [13], in the case of the Laguerre measure, and assuming $k \geqslant n + 1$ Kronrod nodes τ_μ^* in (1.1), expand $L_n\pi_k^*$ in Laguerre polynomials L_j. All these methods require three distinct phases to obtain (1.1): The computation of the appropriate polynomial, say π_{n+1}^*, finding the zeros of π_{n+1}^*, and computing the weights σ_ν, σ_μ^*. An entirely different approach is taken by Kautsky and Elhay [15] and Elhay and Kautsky [5], who compute the nodes τ_μ^* as eigenvalues of a certain matrix derived by matrix decomposition methods—an approach which extends the well-known method of Golub and Welsch [12] for ordinary Gaussian quadratures and its extension by Golub and Kautsky [11]. The weights are then obtained using general methods for constructing interpolatory quadrature rules [14], [6].

Here we propose to compute (1.1) directly by solving a set of nonlinear equations that express the exactness of (1.1) for a given set of $3n + 2$ polynomials. These polynomials are chosen so as to generate a well-conditioned problem. The respective system of nonlinear equations is solved by Newton's method, careful attention being given to the choice of initial approximations and to monitoring the progress of the iteration. We make no claims for our method to be superior in any way to other methods, but merely demonstrate its feasibility and stability. It would indeed be interesting to undertake a detailed comparative study of the various methods now in use.

While aiming directly at the unknown quantities is certainly a virtue if our method is successful, it is less than satisfactory otherwise, since no information about π_{n+1}^* is generated when the method fails. Nevertheless, if one wishes to examine the polynomial π_{n+1}^*, one can express it in terms of the orthogonal polynomials $\{\pi_k(\cdot; d\sigma)\}$ and obtain the coefficients by solving a triangular system of linear equations.

The implementation of Newton's method for computing the Gauss-Kronrod rule (1.1) is discussed in Section 2. In Section 3 we study the condition of the underlying problem. Section 4 deals with the computation of the polynomial π_{n+1}^*. Examples will be given in Section 5, and numerical results for $d\sigma(t) = t^\alpha \ln(1/t)\, dt$ on $[0, 1]$, $\alpha = 0, \pm \frac{1}{2}$, are tabulated in the supplements section at the end of this issue.

For additional questions related to Gauss-Kronrod quadrature we refer the reader to surveys by Monegato [20], [21].

2. The Computation of Gauss-Kronrod Rules by Newton's Method. The Gaussian nodes τ_ν for the measure $d\sigma$ can be computed by well-known methods; see, e.g., [8, p. 290]. We assume therefore that they are available. For a given system of monic polynomials $\{p_k(\cdot)\}$, with $\deg p_k = k$, $k = 0, 1, 2, \ldots$, we further assume that the

first $3n + 2$ modified moments of $d\sigma$,

$$m_k = \int_{\mathbf{R}} p_k(t)\, d\sigma(t), \qquad k = 0,1,\ldots,3n+1, \tag{2.1}$$

are known. The system of nonlinear equations defining the Gauss-Kronrod formula (1.1) then is

$$\sum_{\nu=1}^{n} \sigma_\nu p_k(\tau_\nu) + \sum_{\mu=1}^{n+1} \sigma_\mu^* p_k(\tau_\mu^*) = m_k, \qquad k = 0,1,\ldots,3n+1. \tag{2.2}$$

We propose to solve this system for the $3n + 2$ unknowns τ_μ^*, σ_ν, σ_μ^* by Newton's method. A number of practical issues need to be addressed.

First the choice of polynomials p_k. We assume that they satisfy a three-term recurrence relation,

$$\begin{aligned} p_{-1}(t) &= 0, \qquad p_0(t) = 1, \\ p_{k+1}(t) &= (t - a_k)p_k(t) - b_k p_{k-1}(t), \qquad k = 0,1,2,\ldots, \end{aligned} \tag{2.3}$$

with known coefficients a_k, b_k. This makes the evaluation of these polynomials, and of their derivatives, which is required in the computation of the left-hand side of the system (2.2) and its Jacobian, easy and straightforward. If, in addition, the polynomials $\{p_k\}$ are orthogonal with respect to some given measure $ds(t)$, then this computation is also numerically stable. If $d\sigma$ is one of the classical measures, the simplest choice is $p_k(\cdot) = \pi_k(\cdot; d\sigma)$, the corresponding recursion coefficients $a_k = \alpha_k(d\sigma)$, $b_k = \beta_k(d\sigma)$ then being explicitly known; the modified moments become

$$m_k = \int_{\mathbf{R}} \pi_k(t; d\sigma)\, d\sigma(t) = \beta_0 \delta_{0,k}, \qquad k = 0,1,2,\ldots, \tag{2.4}$$

where $\beta_0 = \int_{\mathbf{R}} d\sigma(t)$ and $\delta_{0,k}$ is the Kronecker delta, $\delta_{0,0} = 1$, $\delta_{0,k} = 0$ if $k > 0$. For nonclassical measures $d\sigma$, the choice of p_k is usually dictated by the necessity of being able to compute the modified moments (2.1).

The next important issue is the computation of the initial approximations for the Kronrod nodes τ_μ^* and for the weights σ_ν, σ_μ^*. Since we are interested only in Gauss-Kronrod formulae with nodes in $[a, b]$ and with positive weights σ_μ^*, we can assume the interlacing property (1.3). This suggests as initial approximations $\mathring{\tau}_\mu^*$, $2 \leqslant \mu \leqslant n$, the midpoints

$$\mathring{\tau}_\mu^* = \tfrac{1}{2}(\tau_{\mu-1} + \tau_\mu), \qquad \mu = 2,3,\ldots,n, \tag{2.5}$$

between the Gaussian nodes $\tau_{\mu-1}$ and τ_μ. The choice of the initial approximations $\mathring{\tau}_1^*$ and $\mathring{\tau}_{n+1}^*$ is less obvious. If the endpoint b is finite, we select a number of trial values $\mathring{\tau}_1^*$ equally spaced between τ_1 and b. If a is also finite, we do the same for $\mathring{\tau}_{n+1}^*$ in the interval (a, τ_n) and let both $\mathring{\tau}_{n+1}^*$ and $\mathring{\tau}_1^*$ move inward simultaneously, or, if necessary, let them move independently from one another. If an endpoint, say b, is infinite, we select $\mathring{\tau}_1^* = \tau_1 + (\tau_1 - \tau_2)$, or try a number of values $\mathring{\tau}_1^*$ equally spaced between τ_1 and, say, $\tau_1 + 2(\tau_1 - \tau_2)$. For each set of initial approximations $\mathring{\tau}_\mu^*$ we compute corresponding approximations $\mathring{\sigma}_\nu$, $\mathring{\sigma}_\mu^*$ to the weights by solving the first $2n + 1$ equations in (2.2), where τ_μ^* is replaced by $\mathring{\tau}_\mu^*$. Since the matrix of this system forms part of the Jacobian matrix used in the first Newton step, the only overhead of this computation is the solution of the linear system.

Each Newton step is monitored as to the location of the iterates of τ_μ^*. If at any stage one of these iterates falls outside the interval $[a, b]$ (if either a or b is finite), the iteration is terminated and restarted with a new set of initial approximations. The same action is taken if the number of Newton iterates exceeds a preset limit. If none of the initial approximations leads to a convergent process, the attempt of computing (1.1) is declared a failure. This is usually an indication (not a proof!) that the desired Gauss-Kronrod rule does not exist.

If $d\sigma(t) = d\sigma(-t)$ is an even measure and the support of $d\sigma$ is symmetric with respect to the origin, then both the Gaussian nodes τ_ν and the Kronrod nodes τ_μ^* are located symmetrically with respect to the origin, and weights corresponding to symmetric nodes are equal. As a result, (2.2) is trivially true if $p_k(t)$ is an odd polynomial. If we choose for $\{p_k\}$ a system of polynomials satisfying

$$p_k(-t) = (-1)^k p_k(t), \qquad k = 0, 1, 2, \ldots, \tag{2.6}$$

the system (2.2), therefore, is equivalent to the system

$$\sum_{\nu=1}^{n/2} \sigma_\nu p_{2k}(\tau_\nu) + \sum_{\mu=1}^{n/2} \sigma_\mu^* p_{2k}(\tau_\mu^*) + \frac{1}{2}\sigma_{(n/2)+1}^* p_{2k}(0) = \frac{1}{2} m_{2k}, \tag{2.7e}$$

$$k = 0, 1, \ldots, 3n/2,$$

if n is even, and to the system

$$\sum_{\nu=1}^{[n/2]} \sigma_\nu p_{2k}(\tau_\nu) + \frac{1}{2}\sigma_{[n/2]+1} p_{2k}(0) + \sum_{\mu=1}^{[n/2]+1} \sigma_\mu^* p_{2k}(\tau_\mu^*) = \frac{1}{2} m_{2k}, \tag{2.7o}$$

$$k = 0, 1, \ldots, (3n+1)/2,$$

if n is odd. This in effect reduces the size of the problem by a factor of 2.

3. The Condition of the Underlying Problem. Let $m^T = [m_0, m_1, \ldots, m_{3n+1}]$ be the vector of modified moments, and $\gamma^T = [\sigma_1, \ldots, \sigma_n, \sigma_1^*, \ldots, \sigma_{n+1}^*, \tau_1^*, \ldots, \tau_{n+1}^*]$ the vector of the weights and Kronrod nodes of the Gauss-Kronrod formula (1.1). The procedure of Section 2 is an attempt of carrying out the nonlinear map

$$G_n: \mathbf{R}^{3n+2} \to \mathbf{R}^{3n+2} \qquad m \to \gamma,$$

where the Gauss-Kronrod formula is assumed to have real nodes. We now wish to examine the sensitivity of the map G_n to perturbations in the modified moments. The development parallels the treatments given for Gaussian formulae in Gautschi [8], [9]; see also Gautschi [10, Section 5].

We assume that the polynomials $\{p_k\}$ defining the modified moments are orthogonal on the real line with respect to some measure ds. The support of this measure normally coincides with the support of $d\sigma$, but does not have to. We define normalized modified moments by

$$\tilde{m}_k = d_k^{-1} m_k, \qquad d_k^2 = \int_{\mathbf{R}} p_k^2(t)\, ds(t), \tag{3.1}$$

and consider, in place of G_n, the map

$$\tilde{G}_n: \mathbf{R}^{3n+2} \to \mathbf{R}^{3n+2} \qquad \tilde{m} \to \gamma, \tag{3.2}$$

where $\tilde{m}^T = [\tilde{m}_0, \tilde{m}_1, \ldots, \tilde{m}_{3n+1}]$. We analyze the sensitivity of $\tilde{G}_n$ by computing the Frobenius norm of the Jacobian matrix, $J_{\tilde{G}_n}$, of the map $\tilde{G}_n$.

The basic equations can be written in the form

$$\Phi(\gamma) = \tilde{m}, \tag{3.3}$$

where

$$\Phi_k(\gamma) = d_k^{-1}\left\{ \sum_{\nu=1}^{n} \sigma_\nu p_k(\tau_\nu) + \sum_{\mu=1}^{n+1} \sigma_\mu^* p_k(\tau_\mu^*) \right\}, \tag{3.4}$$

$$k = 0, 1, 2, \ldots, 3n+1.$$

Since the map $\tilde{G}_n$ amounts to solving (3.3) for γ, the Jacobian of $\tilde{G}_n$ is the inverse of the Jacobian $\partial\Phi/\partial\gamma$ of Φ,

$$J_{\tilde{G}_n} = (\partial\Phi/\partial\gamma)^{-1}. \tag{3.5}$$

An elementary computation shows that

$$\partial\Phi/\partial\gamma = D^{-1}P\Sigma^*, \tag{3.6}$$

where $D = \operatorname{diag}(d_0, d_1, \ldots, d_{3n+1})$, $\Sigma^* = \operatorname{diag}(1, \ldots, 1, 1, \ldots, 1, \sigma_1^*, \ldots, \sigma_{n+1}^*)$, and

(3.7)

$$P = \begin{bmatrix} p_0(\tau_1) & \cdots & p_0(\tau_n) & p_0(\tau_1^*) & \cdots & p_0(\tau_{n+1}^*) & p_0'(\tau_1^*) & \cdots & p_0'(\tau_{n+1}^*) \\ p_1(\tau_1) & \cdots & p_1(\tau_n) & p_1(\tau_1^*) & \cdots & p_1(\tau_{n+1}^*) & p_1'(\tau_1^*) & \cdots & p_1'(\tau_{n+1}^*) \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ p_{3n+1}(\tau_1) & \cdots & p_{3n+1}(\tau_n) & p_{3n+1}(\tau_1^*) & \cdots & p_{3n+1}(\tau_{n+1}^*) & p_{3n+1}'(\tau_1^*) & \cdots & p_{3n+1}'(\tau_{n+1}^*) \end{bmatrix}.$$

Therefore,

$$J_{\tilde{G}_n} = (\Sigma^*)^{-1}P^{-1}D. \tag{3.8}$$

For the inversion of P, define g_ν, h_μ, k_μ to be the elementary Hermite interpolation polynomials of degree $3n+1$, belonging to the nodes τ_ν and τ_μ^*, defined by

$$\left.\begin{aligned} &g_\nu(\tau_\lambda) = \delta_{\nu\lambda}, \quad \lambda = 1, 2, \ldots, n \\ &g_\nu(\tau_\mu^*) = 0, \quad g_\nu'(\tau_\mu^*) = 0, \qquad \mu = 1, 2, \ldots, n+1 \end{aligned}\right\},$$

$$\nu = 1, 2, \ldots, n,$$

$$\left.\begin{aligned} &h_\mu(\tau_\lambda) = 0, \quad \lambda = 1, 2, \ldots, n \\ &h_\mu(\tau_\nu^*) = \delta_{\mu\nu}, \quad h_\mu'(\tau_\nu^*) = 0, \qquad \nu = 1, 2, \ldots, n+1 \\ &k_\mu(\tau_\lambda) = 0, \quad \lambda = 1, 2, \ldots, n \\ &k_\mu(\tau_\nu^*) = 0, \quad k_\mu'(\tau_\nu^*) = \delta_{\mu\nu}, \qquad \nu = 1, 2, \ldots, n+1 \end{aligned}\right\}, \tag{3.9}$$

$$\mu = 1, 2, \ldots, n+1.$$

Writing

$$g_\nu(t) = \sum_{\rho=1}^{3n+2} a_{\nu\rho}p_{\rho-1}(t), \quad h_\mu(t) = \sum_{\rho=1}^{3n+2} b_{\mu\rho}p_{\rho-1}(t), \quad k_\mu(t) = \sum_{\rho=1}^{3n+2} c_{\mu\rho}p_{\rho-1}(t),$$

it is easily seen that

$$P^{-1} = \begin{bmatrix} A \\ B \\ C \end{bmatrix}, \quad A = [a_{\nu\rho}], \quad B = [b_{\mu\rho}], \quad C = [c_{\mu\rho}]. \tag{3.10}$$

By a computation similar to the one in [8, pp. 303–304] one finds from (3.8) and (3.10) that the Frobenius norm of $J_{\tilde{G}_n}$ is given by

$$\|J_{\tilde{G}_n}\|_F = \left\{ \int_{\mathbf{R}} \left[\sum_{\nu=1}^{n} g_\nu^2(t) + \sum_{\mu=1}^{n+1} \left(h_\mu^2(t) + \frac{1}{\sigma_\mu^{*2}} k_\mu^2(t) \right) \right] ds(t) \right\}^{1/2}. \tag{3.11}$$

Its magnitude, therefore, is critically influenced by the magnitude of the polynomial

$$f_n(t) = \sum_{\nu=1}^{n} g_\nu^2(t) + \sum_{\mu=1}^{n+1} \left(h_\mu^2(t) + \frac{1}{\sigma_\mu^{*2}} k_\mu^2(t) \right) \tag{3.12}$$

on the support of ds. The degree of f_n is $6n + 2$. The integral in (3.11) can therefore be computed exactly (up to rounding errors) by a $(3n + 2)$-point Gaussian quadrature rule belonging to the measure ds.

Explicit forms of the polynomials g_ν, h_μ, k_μ can easily be given in terms of the fundamental Lagrange polynomials

$$l_\nu(t) = \prod_{\substack{\lambda=1 \\ \lambda \neq \nu}}^{n} \frac{t - \tau_\lambda}{\tau_\nu - \tau_\lambda}, \qquad l_\mu^*(t) = \prod_{\substack{\lambda=1 \\ \lambda \neq \mu}}^{n+1} \frac{t - \tau_\lambda^*}{\tau_\mu^* - \tau_\lambda^*}$$

belonging to the nodes τ_ν and τ_μ^*, respectively. One obtains

$$g_\nu(t) = l_\nu(t) \left[\frac{\pi_{n+1}^*(t)}{\pi_{n+1}^*(\tau_\nu)} \right]^2, \qquad \nu = 1, 2, \ldots, n,$$

$$h_\mu(t) = \frac{\pi_n(t)}{\pi_n(\tau_\mu^*)} \left[l_\mu^*(t) \right]^2 \left\{ 1 - (t - \tau_\mu^*) \left[\frac{\pi_n'(\tau_\mu^*)}{\pi_n(\tau_\mu^*)} + 2 l_\mu^{*\prime}(\tau_\mu^*) \right] \right\}, \tag{3.13}$$

$$\mu = 1, 2, \ldots, n + 1,$$

$$k_\mu(t) = \frac{\pi_n(t)}{\pi_n(\tau_\mu^*)} \left[l_\mu^*(t) \right]^2 (t - \tau_\mu^*), \qquad \mu = 1, 2, \ldots, n + 1,$$

where $\pi_n(\cdot) = \pi_n(\cdot; d\sigma)$ and $\pi_{n+1}^*(t) = \prod_{\lambda=1}^{n+1}(t - \tau_\lambda^*)$. We also note the following properties of f_n, which follow directly from (3.9) and (3.12),

$$\begin{aligned} &f_n(t) > 0 \quad \text{for all } t \in \mathbf{R}, \\ &f_n(\tau_\nu) = 1, \quad f_n'(\tau_\nu) = 2 g_\nu'(\tau_\nu), \qquad \nu = 1, 2, \ldots, n, \\ &f_n(\tau_\mu^*) = 1, \quad f_n'(\tau_\mu^*) = 0, \qquad \mu = 1, 2, \ldots, n + 1. \end{aligned} \tag{3.14}$$

These conditions, of course, are not sufficient to determine the polynomial f_n. There are $2n + 1$ degrees of freedom left, which allow f_n considerable room for movement.

4. Computation of the Polynomial π_{n+1}^*. Expressing the polynomial π_{n+1}^* in terms of the orthogonal polynomials $\pi_k(\cdot) = \pi_k(\cdot; d\sigma)$,

$$\pi_{n+1}^*(t) = \pi_{n+1}(t) + c_0 \pi_n(t) + c_1 \pi_{n-1}(t) + \cdots + c_n \pi_0(t), \tag{4.1}$$

and replacing the powers t^i in (1.2) by the polynomials $\pi_i(t)$, one obtains the conditions

$$\int_{\mathbf{R}} \left[\pi_{n+1}(t) + \sum_{k=0}^{n} c_k \pi_{n-k}(t) \right] \pi_n(t) \pi_i(t)\, d\sigma(t) = 0, \qquad i = 0, 1, \ldots, n,$$

hence the linear system

$$\sum_{k=0}^{n} a_{ik}c_k = b_i, \qquad i = 0,1,\ldots,n, \tag{4.2}$$

for the coefficients c_k, where

$$\begin{aligned} a_{ik} &= \int_{\mathbf{R}} \pi_i(t)\pi_{n-k}(t)\pi_n(t)\,d\sigma(t), \qquad i,k = 0,1,\ldots,n, \\ b_i &= -\int_{\mathbf{R}} \pi_i(t)\pi_{n+1}(t)\pi_n(t)\,d\sigma(t), \qquad i = 0,1,\ldots,n. \end{aligned} \tag{4.3}$$

By orthogonality, $a_{ik} = 0$ if $i < k$, so that the matrix $A = [a_{ik}]$ is lower triangular, and $a_{ii} = \int_{\mathbf{R}} \pi_n^2(t)\,d\sigma(t) > 0$, so that A is nonsingular. The solution of (4.2), therefore, can be effected by forward substitution.

The coefficients a_{ik} and $b_i = -a_{i,-1}$ satisfy a two-dimensional recursion relation, which could be used for their computation (see [2]). Noting, however, that the integrands in (4.3) are polynomials of degree at most equal to $3n + 1$, we can also use m-point Gauss-Christoffel quadrature relative to the measure $d\sigma$, with $m = [(3n + 3)/2]$, to compute a_{ik} and b_i. This might be preferable, since it requires nothing beyond standard software.

While this procedure of generating π_{n+1}^* is similar to Kronrod's original method, it is significantly more stable, since the use of powers as a polynomial basis is completely avoided.

5. Examples. It is known that for $d\sigma(t) = (1 - t^2)^{\lambda - 1/2}\,dt$ on $[-1,1]$ all Gauss-Kronrod formulae exist if $0 \leqslant \lambda \leqslant 2$. Furthermore, the interlacing property (1.3) holds and $\sigma_\mu^* > 0$ for $\mu = 1,2,\ldots,n+1$ (Monegato [17]). If $0 \leqslant \lambda \leqslant 1$, one has in addition $\sigma_\nu > 0$ for $\nu = 1,2,\ldots,n$ (Monegato [18]). Our first example deals with the case $\lambda = \frac{1}{2}$, i.e., with the Legendre measure. All computations reported were done on the CDC 6500 computer in single precision (machine precision $\approx 3.55 \times 10^{-15}$), unless noted otherwise.

Example 5.1. $d\sigma(t) = dt$ on $[-1,1]$.

Taking advantage of symmetry, we apply Newton's method to the system (2.7), using for p_{2k} the (monic) Legendre polynomials of degree $2k$. The required modified moments are then given by (2.4). We had no difficulty with convergence. By symmetry, only *one* "trial" initial approximation, $\mathring{\tau}_1^*$, is needed, which was programmed to move in nine equal steps of length $h = (1 - \tau_1)/10$ from $1 - h$ to $\tau_1 + h$. Convergence was invariably achieved for the first choice of $\mathring{\tau}_1^*$. Moreover, the problem, suitably scaled, turns out to be extremely stable. In the first four columns of Table 5.1 we report on the number of iterations required for 12 decimal place accuracy, the maximum of $f_n(t)$ (cf. Eq. (3.12)) on $[-1,1]$ and the value of $\|J_{\tilde{G}_n}\|_F$ (cf. Eq. (3.11)) for $n = 5$, 10, 20, 40, 80. The maximum of $f_n(t)$—an even function of t—is typically assumed between τ_2 and τ_2^*, if n is even, there being a couple of smaller maxima on either side of it. If n is odd, the maximum seems to occur at $t = 1$. Through most of the interval $(-1,1)$, however, f_n remains $\leqslant 1$.

TABLE 5.1

Performance and stability characteristics of Newton's method for generating the $(2n+1)$*-point Gauss-Kronrod formula with* $d\sigma(t) = dt$ *on* $[-1,1]$.

n	#iter.	$\|f_n\|_\infty$	$\|J_{\tilde{G}_n}\|_F$	cond_1	cond_2	cond_1 (scaled)	cond_2 (scaled)
5	6	1.126	1.293	1.4(3)	3.3(4)	1.2(1)	1.4(1)
10	6	2.456	1.397	1.5(6)	5.2(8)	1.8(1)	2.3(1)
20	6	2.520	1.333	1.5(12)	5.3(17)	4.1(1)	4.8(1)
40	6	2.535	1.310	1.6(24)	5.8(35)	6.6(1)	7.7(1)
80	6	2.540	1.302	—	—	1.3(2)	1.7(2)

The linear systems of equations for determining the initial approximations $\mathring{\sigma}_\nu$, $\mathring{\sigma}_\mu^*$ for the weights, as well as the Jacobian matrices in Newton's method, appear to become rapidly ill-conditioned as n increases. Typical condition number estimates (furnished by the LINPACK routine SGECO; cf. [4, Chapter 1]) for the former are shown in the fifth column of Table 5.1, while those for the latter are shown in the sixth column. (Numbers in parentheses indicate decimal exponents.) In spite of the large condition numbers, numerical difficulties were not observed, except in the case $n = 80$, when the computation was aborted due to an arithmetic error. We believe that the apparent ill-conditioning is caused by the use of monic polynomials p_{2k} in (2.7); their L_2-norm goes to zero rather quickly,

$$\|p_{2k}\|_2 = \frac{2^{2k}(2k)!^2}{(4k)!}\sqrt{\frac{2}{4k+1}} \sim \sqrt{\pi}\,2^{-2k} \quad \text{as } k \to \infty,$$

thereby introducing a systematic diminution of the rows down the matrices. If the row involving p_{2k} is scaled by dividing it by $2^{2k}(2k)!^2/(4k)!$, the condition numbers indeed become much more reasonable (the solutions remaining the same); they are shown in the last two columns of Table 5.1.

Example 5.2. $d\sigma(t) = \ln(1/t)\,dt$ on $[0,1]$.

It appears that this measure also admits Gauss-Kronrod formulae for all n, satisfying the interlacing property (1.3) and having all weights positive. A summary of our numerical experience with Newton's method is given in Table 5.2; it contains information analogous to the one given in Table 5.1 for Example 5.1.

TABLE 5.2

Newton's method for Gauss-Kronrod formulae with $d\sigma(t) = \ln(1/t)\,dt$ *on* $[0,1]$.

n	#iter.	$\|f_n\|_\infty$	$\|J_{\tilde{G}_n}\|_F$	cond_1	cond_2	cond_1 (scaled)	cond_2 (scaled)
5	6	2.90(4)	12.14	2.0(6)	6.9(9)	5.8(1)	2.7(3)
10	6	4.09(5)	24.35	2.2(12)	7.5(18)	2.8(1)	1.6(4)
20	6	5.77(6)	47.43	2.4(24)	8.2(36)	9.8(2)	1.0(5)
40	6	8.86(7)	94.59	—	—	3.8(3)	6.4(5)

We have used modified moments with respect to the (monic) shifted Legendre polynomials, $p_k(t) = [k!^2/(2k)!]P_k^*(t)$; they are known to be (cf., e.g., Gautschi [7])

$$m_0 = 1, \qquad m_k = \int_0^1 p_k(t)\ln(1/t)\,dt = \frac{k!^2}{(2k)!}\,\frac{(-1)^k}{k(k+1)}, \qquad k = 1,2,\ldots.$$

Row scaling of the matrices was performed through division by $k!^2/(2k)!$ (of the row numbered $k + 1$).

The initial approximations $\mathring{\tau}_1^*$ and $\mathring{\tau}_{n+1}^*$ were programmed to first move inward symmetrically in nine steps of length $h = (1 - \tau_1)/10$ and $h' = \tau_n/10$, respectively, and if this did not work, $\mathring{\tau}_1^*$ was varied independently over the same set of points for each fixed $\mathring{\tau}_{n+1}^*$. Convergence, in general, was achieved for the very first choice of $\mathring{\tau}_1^*$ and $\mathring{\tau}_{n+1}^*$, i.e., for $\mathring{\tau}_1^* = 1 - h$ and $\mathring{\tau}_{n+1}^* = h'$, except when n is small, for example, $n = 1$ and $n = 3$, in which cases convergence was realized when $\mathring{\tau}_{n+1}^* = h'$ and $\mathring{\tau}_1^* = 1 - 4h$ (for $n = 1$), $\mathring{\tau}_1^* = 1 - 2h$ (for $n = 3$).

The polynomial $f_n(t)$ invariably assumes its global maximum at $t = 1$, has a few much smaller relative maxima between the first few neighboring nodes τ_μ^* and τ_ν, and then settles down to magnitudes around 1 for the remaining portion of the interval $[0, 1]$. The condition of the problem, though slightly worse than in Example 5.1, is still remarkably good.

Numerical results for the nodes and weights of the $(2n + 1)$-point Gauss-Kronrod formula for $n = 5(5)25$ can be found in Table S.1 of the supplements section at the end of this issue. They have been computed in double precision to an accuracy of 25 decimal places after the decimal point. As the results are displayed in D-format, some of the end figures may not be reliable in those numbers that are much smaller than 1.

We used Example 5.2 to further experiment with alternative choices of initial approximations. In particular, we examined how inaccuracies in individual initial approximations affect the speed of convergence. To obtain a basis for meaningful comparison, we first obtained "reference" values for the number of iterations required when all initial approximations are at the same level of accuracy. This was achieved by imposing on the "exact" results for σ_ν, σ_μ^*, τ_μ^* (computed to 12 decimal digits) a random perturbation at level ε, i.e., by taking $\mathring{\sigma}_\nu = \sigma_\nu(1 + r_\nu\varepsilon)$, $\mathring{\sigma}_\mu^* = \sigma_\mu^*(1 + r_\mu^*\varepsilon)$, $\mathring{\tau}_\mu^* = \tau_\mu^*(1 + s_\mu^*\varepsilon)$, where r_ν, r_μ^*, s_μ^* are random numbers from $[-1, 1]$. The results for $\varepsilon = 10^{-2}$, 10^{-5}, 10^{-8}, and 10^{-11} are shown in Table 5.3. (For $\varepsilon = 10^{-2}$ and $n = 40$, Newton's method did not converge within 20 iterations.)

TABLE 5.3

The number of iterations required for initial approximations at accuracy level ε.

ε	$n = 5$	$n = 10$	$n = 20$	$n = 40$
10^{-2}	6	6	5	—
10^{-5}	3	3	3	4
10^{-8}	2	2	2	2
10^{-11}	2	2	2	2

TABLE 5.4

The number of iterations required when two pairs of initial approximations (with indices μ and $n + 2 - \mu$) are inaccurate.

ε	$\mu = 1$				$\mu \approx n/4$				$\mu = n/2$			
	$n = 5$	$n = 10$	$n = 20$	$n = 40$	$n = 5$	$n = 10$	$n = 20$	$n = 40$	$n = 5$	$n = 10$	$n = 20$	$n = 40$
10^{-2}	5	4	6	6	5	4	6	5	4	4	5	6
10^{-5}	3	3	3	4	3	3	3	3	3	3	3	3
10^{-8}	2	2	2	2	2	2	2	2	2	2	2	2
10^{-11}	2	2	2	2	2	2	2	2	2	2	2	2

We now contrast this with the case in which all initial approximations are at the accuracy level $\frac{1}{2}10^{-12}$ of the initially computed results, except for two pairs of Kronrod nodes and weights (situated symmetrically with respect to the midpoint of the interval [0, 1]), which are randomly perturbed at level ε. Choosing the inaccurate pairs $\mathring{\tau}_\mu^*$, $\mathring{\sigma}_\mu^*$ to be those corresponding to $\mu = 1$, $\mu \approx n/4$, and $\mu \approx n/2$ (and to the symmetric indices $n + 2 - \mu$), we observed the results shown in Table 5.4.

Comparing Tables 5.3 and 5.4, we note some improvement, particularly for $\mu \approx n/2$, in the case $\varepsilon = 10^{-2}$, when only two pairs of initial approximations are inaccurate (though for $n = 20$ there are two instances of deterioration), but in all other cases the performance of Newton's iteration is practically the same. This seems to suggest that it is the maximum relative error in the initial approximations (usually associated with a Kronrod or Gauss node near the end of the interval) which determines the speed of convergence.

The choice of initial approximations proposed in Section 2 leads to initial (relative) errors that are reasonably small for "interior" nodes, but comparatively larger near the "boundary". Specifically, if we regard the three Kronrod nodes nearest to each of the endpoints of [0, 1], and the two Gauss nodes between them, as belonging to the "boundary", and all others to the "interior", then the relative errors of the initial approximations in our scheme range for $n = 10$, 20, 40 respectively from 2.0(−3) to 9.5(−2), 2.4(−5) to 5.5(−2), and 4.3(−6) to 2.9(−2) in the interior, and from 4.3(−3) to 5.4(−1), 1.3(−3) to 5.6(−1), and 3.3(−4) to 5.7(−1), respectively, at the boundary. The relatively large number of 6 iterations reported in Table 5.2 appears to be due to the large maximum error of the initial approximations in the boundary zones.

Attempts to improve the initial approximations for σ_ν by using, for example, $\sigma_\nu = \frac{1}{2}\sigma_\nu^{(n)}$,** where $\sigma_\nu^{(n)}$ are the Christoffel numbers for $d\sigma$, and by obtaining the remaining initial approximations σ_μ^* from a reduced system (2.2) of $n + 1$ linear equations, do not speed up Newton's iteration (in fact, require 7 iterations, instead of 6, when $n = 5$ and $n = 10$), precisely because of the initial approximations in the boundary zones remaining at the same low accuracy level.

Example 5.3. $d\sigma(t) = t^\alpha \ln(1/t)\, dt$ on [0, 1], $\alpha = \pm \frac{1}{2}$.

Modified moments with respect to the shifted Legendre polynomials are again available (Gautschi [7]) and suggest the same scaling as in Example 5.2. Results for

** This approximation was proposed to us by the referee.

TABLE 5.5

Newton's method for Gauss-Kronrod formulae with $d\sigma(t) = t^{1/2}\ln(1/t)\,dt$ *on* $[0,1]$.

n	#iter.	$\|f_n\|_\infty$	$\|J_{\tilde{G}_n}\|_F$	cond_1 (scaled)	cond_2 (scaled)
5	6	1.03(4)	7.542	3.8(3)	7.8(4)
10	6	1.35(5)	14.64	7.3(4)	1.0(6)
20	6	2.06(6)	29.60	5.2(5)	1.4(7)
40	6	3.40(7)	61.04	1.4(7)	3.0(8)

TABLE 5.6

Newton's method for Gauss-Kronrod formulae with $d\sigma(t) = t^{-1/2}\ln(1/t)\,dt$ *on* $[0,1]$.

n	#iter.	$\|f_n\|_\infty$	$\|J_{\tilde{G}_n}\|_F$	cond_1 (scaled)	cond_2 (scaled)
4	7	9.78(6)	272.21	1.3(2)	9.0(5)
8	9	3.66(8)	889.01	2.0(3)	1.3(7)
16	9	1.52(10)	2961.5	6.3(3)	2.0(8)
32	—	6.56(11)	9907.2	8.8(3)	3.1(9)

$\alpha = \frac{1}{2}$ are summarized in Table 5.5. (The computation was done in double precision, the number of iterations referring again to 12 decimal place accuracy.) The performance of Newton's method is similar as in Example 5.2, except for the (scaled) matrices now being more ill-conditioned. The ill-conditioning of the Jacobian matrices is still worse in the case $\alpha = -\frac{1}{2}$, as can be seen from Table 5.6. For this value of α the independent variation of the starting approximations $\mathring{\tau}_1^*$, $\mathring{\tau}_{n+1}^*$ proved to be rather essential, since convergence was *never* achieved for the first choices of these starting values. This is in contrast to the case $\alpha = \frac{1}{2}$, where the first choice of $\mathring{\tau}_1^*$ and $\mathring{\tau}_{n+1}^*$ *always* worked.

When $\alpha = -\frac{1}{2}$, Newton's method could not be made to converge for $n = 32$, using the implementation described in Section 2. The difficulty, we believe, is caused by the smallest Kronrod node being almost equal to zero. Computing (in double precision) π_{33}^* by the procedure of Section 4, and applying Newton's method to π_{33}^*, we find $\tau_{33}^* = 3.05867\ldots \times 10^{-9}$. Using all zeros of π_{33}^* computed in this way as initial approximations to Newton's method, and lowering the accuracy requirement to 20 decimal places, indeed restores convergence and yields the data for $n = 32$ in Table 5.6 after 1 iteration.

Nonconvergence (in the case $\alpha = -\frac{1}{2}$) was also observed for odd values of n, this time because of the presence of negative Kronrod nodes. When $n = 1$, for example, one computes directly $\pi_2^*(t) = t^2 - (198/343)t - (3671/117649)$, which has the zeros $\tau_1^* = .627023\ldots$ and $\tau_2^* = -.0497636\ldots$. We verified that for all odd $n < 32$ the polynomial π_{n+1}^* has exactly one negative zero, while all other zeros are between 0 and 1.

Numerical results for $\alpha = \frac{1}{2}$, $n = 5(5)25$, computed in double precision, are given in Table S.2 and for $\alpha = -\frac{1}{2}$, $n = 4(4)24$, in Table S.3 of the supplements section at the end of this issue.

Dipartimento di Matematica
Politecnico Milano
Piazza Leonardo da Vinci, 32
20133 Milano, Italy

Department of Computer Sciences
Purdue University
West Lafayette, Indiana 47907

Dipartimento di Matematica
Politecnico Milano
Piazza Leonardo da Vinci, 32
20133 Milano, Italy

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