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A Family of Gauss-Kronrod Quadrature Formulae*

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Dedicated with affection to Dick Varga on his 60th birthday

Abstract. We show, for each $n \geq 1$, that the $(2n+1)$-point Kronrod extension of the n-point Gaussian quadrature formula for the measure

$$d\sigma_\gamma(t) = (1+\gamma)^2(1-t^2)^{1/2}dt/((1+\gamma)^2 - 4\gamma t^2), \qquad -1 < \gamma \leq 1,$$

has the properties that its $n+1$ Kronrod nodes interlace with the n Gauss nodes and all its $2n+1$ weights are positive. We also produce explicit formulae for the weights.

1. Introduction. Given a positive measure $d\sigma$ on the real line, whose moments all exist, a quadrature rule

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

is called a *Gauss-Kronrod formula* if $\tau_\nu = \tau_\nu^{(n)}$ are the Gaussian nodes for the measure $d\sigma$, i.e., the zeros of the nth degree orthogonal polynomial $\pi_n(\cdot) = \pi_n(\cdot; d\sigma)$, and the nodes $\tau_\mu^* = \tau_\mu^{*(n)}$ and weights $\sigma_\nu = \sigma_\nu^{(n)}$, $\sigma_\mu^* = \sigma_\mu^{*(n)}$ are chosen so as to maximize the degree of exactness of (1.1); thus, $R_n(f) = 0$ for all $f \in \mathbf{P}_{3n+1}$ at least. It is well known (see, e.g., the survey in [1]) that the "Kronrod nodes" τ_μ^* must be the zeros of the polynomial $\pi_{n+1}^*(\cdot; d\sigma)$ of degree $n+1$ orthogonal to all lower-degree polynomials relative to the (sign-variable) measure $d\sigma^*(t) = \pi_n(t)d\sigma(t)$:

$$\int_{\mathbf{R}} \pi_{n+1}^*(t; d\sigma)p(t)\pi_n(t; d\sigma)d\sigma(t) = 0, \quad \text{all } p \in \mathbf{P}_n. \tag{1.2}$$

While π_{n+1}^* (assumed monic) is known to exist uniquely, there is no assurance, in general, that its zeros τ_μ^* are all real and simple, and distinct from the Gaussian nodes τ_ν.

In practice, it is particularly desirable to have the following two properties satisfied:

(i) the *interlacing* property,

$$-\infty < \tau_{n+1}^{*(n)} < \tau_n^{(n)} < \tau_n^{*(n)} < \cdots < \tau_2^{*(n)} < \tau_1^{(n)} < \tau_1^{*(n)} < \infty, \tag{1.3}$$

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with all nodes contained in the support interval of $d\sigma$, and

(ii) the *positivity* of all weights,

$$\sigma_\nu^{(n)} > 0, \qquad \nu = 1, 2, \ldots, n; \qquad \sigma_\mu^{*(n)} > 0, \qquad \mu = 1, 2, \ldots, n+1. \tag{1.4}$$

(The inequalities $\sigma_\mu^* > 0$ are actually equivalent to (1.3); see Monegato [4].) Only one family of measures $d\sigma$ is presently known for which both properties (i) and (ii) hold for all $n \geq 1$, namely the Gegenbauer measure $d\sigma^\lambda(t) = (1-t^2)^{\lambda - 1/2}\,dt$ on $(-1,1)$. For this measure, (1.3) (with $-1 \leq \tau_{n+1}^*$ and $\tau_1^* \leq 1$) has been established by Szegö [7] for $0 \leq \lambda \leq 2$, and (1.4) by Monegato [5] for $0 \leq \lambda \leq 1$. In this note we show that the family of measures

$$d\sigma_\gamma(t) = (1+\gamma)^2 \frac{(1-t^2)^{1/2}}{(1+\gamma)^2 - 4\gamma t^2}\,dt \quad \text{on } (-1,1), \quad -1 < \gamma \leq 1, \tag{1.5}$$

already considered by Geronimus [3] and Monegato [6], also has these same properties, i.e., (1.3) (with $-1 \leq \tau_{n+1}^*$ and $\tau_1^* \leq 1$) and (1.4) both hold for all $n \geq 1$. In addition, as is known (Monegato [6, p. 146]), the degree of precision of (1.1) for $d\sigma = d\sigma_\gamma$ is exceptionally high, namely, if $n > 1$, exactly $4n-1$ and $4n+1$ when $\gamma \neq 0$ and $\gamma = 0$, respectively, and 5 if $n = 1$.

Note that the restriction $-1 < \gamma \leq 1$ in (1.5) is a natural one, since the measure is $(1-t^2)^{1/2}\,dt/(1-\mu t^2)$, $\mu = 4\gamma/(1+\gamma)^2$, and μ runs through all admissible values $-\infty < \mu \leq 1$ as γ varies from -1 to 1.

In a sense, the results obtained here for the Geronimus measure (1.5) are more pleasing than those presently known for the Gegenbauer measure. Not only do we have higher degree of accuracy and explicit formulae, but our results cover an entire class of measures, in contrast to those for the Gegenbauer measure, which are partial at best. See, in this connection, the numerical work in [2].

The proofs of (i) and (ii) for the measure (1.5) are facilitated by the fact that both (monic) polynomials $\pi_n(\cdot; d\sigma_\gamma)$ and $\pi_{n+1}^*(\cdot; d\sigma_\gamma)$ are known explicitly,

$$\pi_n(t; d\sigma_\gamma) = 2^{-n}[U_n(t) - \gamma U_{n-2}(t)], \tag{1.6}$$

$$\begin{aligned} \pi_2^*(t; d\sigma_\gamma) &= \tfrac{1}{2}\left[T_2(t) - \tfrac{1}{2}\gamma\right], \\ \pi_{n+1}^*(t; d\sigma_\gamma) &= 2^{-n}[T_{n+1}(t) - \gamma T_{n-1}(t)], \qquad n \geq 2. \end{aligned} \tag{1.6*}$$

(Cf. Monegato [6, p. 146]; the first relation in (1.6*) is not given in this reference but follows from an elementary computation.) Here, T_m and U_m denote the mth degree Chebyshev polynomials of the first and second kind.

2. Interlacing. If $\gamma = 1$, then $d\sigma_\gamma(t) = (1-t^2)^{-1/2}\,dt$ is the Chebyshev measure of the first kind, that is, a Gegenbauer measure with $\lambda = 0$, so that (1.3) and (1.4) hold. If $\gamma < 1$, it follows from (1.6*) that the zeros of π_{n+1}^* are all in the interior of $[-1,1]$ and are separated by the extreme points of T_{n+1}. As γ is continuously decreased from $\gamma = 1$ to $\gamma = -1$, the only way (1.3) can cease to hold is that for some $\gamma = \gamma_0$, $-1 < \gamma_0 < 1$, the two polynomials π_n, π_{n+1}^* have a common zero τ_0. We now show that this is impossible.

The case $n = 1$ being trivial, we may assume $n \geq 2$. Suppose, then, that τ_0 is a common zero of π_n and π_{n+1}^*,

$$(U_n - \gamma U_{n-2})(\tau_0) = (T_{n+1} - \gamma T_{n-1})(\tau_0) = 0 \quad \text{for } \gamma = \gamma_0. \tag{2.1}$$

It is clear, first of all, that $\tau_0 \neq 0$, since otherwise, one of the two expressions on the left of (2.1) is zero and the other $\pm(1+\gamma) \neq 0$. Furthermore, $U_{n-2}(\tau_0) \neq 0$, $T_{n-1}(\tau_0) \neq 0$. We show only the first inequality; the other is proved similarly. If we had $U_{n-2}(\tau_0) = 0$, then, by (2.1), $U_n(\tau_0) = 0$, and the recurrence formula $U_n(\tau_0) = 2\tau_0 U_{n-1}(\tau_0) - U_{n-2}(\tau_0)$ would imply, since $\tau_0 \neq 0$, that $U_{n-1}(\tau_0) = 0$. This contradicts the well-known fact that two consecutive orthogonal polynomials cannot vanish at the same point.

It now follows from (2.1) that

$$\gamma_0 = \frac{U_n(\tau_0)}{U_{n-2}(\tau_0)} = \frac{T_{n+1}(\tau_0)}{T_{n-1}(\tau_0)},$$

hence

$$\Delta_n := U_n T_{n-1} - U_{n-2} T_{n+1} = 0 \quad \text{at } \tau_0. \tag{2.2}$$

Since $U_m(t)$ and $T_m(t)$ both satisfy

$$y_{m+1} = (4t^2-2)y_{m-1} - y_{m-3},$$

where $m \geq 3$ for T, and $m \geq 2$ for U, there follows, for $n = 3, 4, 5, \ldots$, that

$$\begin{aligned}\Delta_n &= [(4t^2-2)U_{n-2} - U_{n-4}]T_{n-1} - U_{n-2}[(4t^2-2)T_{n-1} - T_{n-3}] \\ &= U_{n-2}T_{n-3} - U_{n-4}T_{n-1} \\ &= \Delta_{n-2},\end{aligned}$$

hence $\Delta_n = \Delta_2$ for n even, and $\Delta_n = \Delta_1$ for n odd. But, for $t = \tau_0 \neq 0$, $\Delta_2 = \Delta_1 = 2\tau_0 \neq 0$, so that $\Delta_n \neq 0$, contrary to (2.2). This proves the interlacing property for $-1 < \gamma \leq 1$ and all $n \geq 1$.

3. Positivity. We actually derive explicit formulae for σ_ν and σ_μ^*, from which positivity can be read off: see Eqs. (3.9), (3.11).

Let $\tau_\nu = \cos\theta_\nu$, $0 < \theta_\nu < \pi$, and assume first $n \geq 2$ and $\tau_\nu \neq 0$, that is, $\theta_\nu \neq \pi/2$. Since $U_{n-2}(\tau_\nu) \neq 0$ (cf. Section 2), we have by (1.6), using $U_{m-1}(\cos\theta) = \sin m\theta / \sin\theta$, that

$$\gamma = \frac{\sin(n+1)\theta_\nu}{\sin(n-1)\theta_\nu} \tag{3.1}$$

for each ν.

It is well known (cf. Monegato [4]) that

$$\sigma_\nu = \lambda_\nu + \frac{\|\pi_n\|^2_{d\sigma_\gamma}}{\pi^*_{n+1}(\tau_\nu)\pi'_n(\tau_\nu)}, \qquad \nu = 1, 2, \ldots, n, \tag{3.2}$$

where $\pi_n(\cdot) = \pi_n(\cdot; d\sigma_\gamma)$ and $\lambda_\nu = \lambda_\nu^{(n)}$ are the Christoffel numbers for $d\sigma_\gamma$; for the latter, we have (see, e.g., [8, Eq. (3.4.7)])

$$\lambda_\nu = -\frac{\|\pi_n\|^2_{d\sigma_\gamma}}{\pi_{n+1}(\tau_\nu)\pi'_n(\tau_\nu)}, \qquad \nu = 1, 2, \ldots, n. \tag{3.3}$$

Putting $t = \cos\theta_\nu$ in (1.6*), and using $T_m(\cos\theta) = \cos m\theta$ and (3.1), one finds

$$\pi^*_{n+1}(\tau_\nu) = -2^{-n}\frac{\sin 2\theta_\nu}{\sin(n-1)\theta_\nu}. \tag{3.4}$$

Similarly, from (1.6), replacing n by $n+1$, one gets after a little computation

$$\pi_{n+1}(\tau_\nu) = -2^{-n-1}\frac{\sin 2\theta_\nu}{\sin(n-1)\theta_\nu}. \tag{3.5}$$

Interestingly, $\pi_{n+1}(\tau_\nu)$ has precisely half the value of $\pi^*_{n+1}(\tau_\nu)$, which, by (3.2) and (3.3), implies that the second term on the right of (3.2) is half as big (in modulus) as the first and of opposite sign. Since $\lambda_\nu > 0$, this already proves $\sigma_\nu > 0$. But we want an explicit formula for σ_ν and therefore proceed with our computation.

We first incorporate the preceding remark in (3.2) and write

$$\sigma_\nu = -\frac{\|\pi_n\|^2_{d\sigma_\gamma}}{\pi^*_{n+1}(\tau_\nu)\pi'_n(\tau_\nu)}. \tag{3.6}$$

Differentiating (1.6) gives

$$\begin{aligned}\cos\theta\cdot\pi_n(\cos\theta) &- \sin^2\theta\cdot\pi'_n(\cos\theta)\\ &= n\pi^*_{n+1}(\cos\theta) + 2^{-n}[\cos(n+1)\theta + \gamma\cos(n-1)\theta].\end{aligned}$$

Now substitute from (3.1) for γ, put $\theta = \theta_\nu$ and use (3.4) to get

$$-\pi^*_{n+1}(\tau_\nu)\pi'_n(\tau_\nu) = 2^{-2n+1}\frac{\cos\theta_\nu}{\sin\theta_\nu \sin^2(n-1)\theta_\nu}[n\sin 2\theta_\nu - \sin 2n\theta_\nu]. \tag{3.7}$$

It remains to calculate the norm of π_n. For this, we use the fact that

$$\|\pi_n\|^2_{d\sigma_\gamma} = \beta_0\beta_1\beta_2\cdots\beta_n,$$

where $\beta_0 = \int_{-1}^1 d\sigma_\gamma(t)$ and β_k are the recursion coefficients in

$$\begin{gathered}\pi_{k+1}(t) = t\pi_k(t) - \beta_k\pi_{k-1}(t), \qquad k = 0,1,2,\ldots,\\ \pi_0(t) = 1, \qquad \pi_{-1}(t) = 0.\end{gathered}$$

An elementary calculation shows that

$$\beta_0 = \frac{\pi}{2}(1+\gamma), \quad \beta_1 = \frac{1}{4}(1+\gamma), \quad \beta_2 = \beta_3 = \cdots = \frac{1}{4}.$$

Therefore,

$$\|\pi_n\|^2_{d\sigma_\gamma} = \frac{\pi}{2}\left(\frac{1+\gamma}{2^n}\right)^2, \qquad n \geq 1, \tag{3.8}$$

or, alternatively, using (3.1) once again,

$$\|\pi_n\|^2_{d\sigma_\gamma} = \pi\cdot 2^{-2n+1}\frac{\sin^2 n\theta_\nu \cos^2\theta_\nu}{\sin^2(n-1)\theta_\nu}, \qquad n \geq 2. \tag{3.8$'$}$$

With (3.7), (3.8′) inserted in (3.6), one obtains

$$\begin{aligned}\sigma_\nu^{(n)} = \frac{\pi}{2}\frac{\sin^2 n\theta_\nu}{n - \sin 2n\theta_\nu/\sin 2\theta_\nu}, &\qquad \nu = 1,2,\ldots,n;\\ &n \geq 2, \quad \nu \neq \frac{n+1}{2} \text{ if } n \text{ is odd.}\end{aligned} \tag{3.9}$$

From this, the positivity $\sigma_\nu > 0$ follows once again, since $U_{n-1}(\cos 2\theta) = \sin 2n\theta/\sin 2\theta < n$ for $0 < \theta < \pi$, $\theta \neq \pi/2$.

It remains to consider the case $\tau_\nu = 0$, i.e., in the ordering (1.3), $\nu = (n+1)/2$, where $n \geq 1$ is odd. By (3.8), and calculating $\pi^*_{n+1}(0)$ and $\pi'_n(0)$ directly, from (3.6) one readily finds

$$(3.9') \qquad \sigma_1^{(1)} = \frac{\pi}{2}\frac{1+\gamma}{2+\gamma}; \quad \sigma_{(n+1)/2}^{(n)} = \frac{\pi}{2}\frac{1+\gamma}{1-\gamma+n(1+\gamma)}, \quad n(\text{odd}) \geq 3.$$

The positivity $\sigma^*_\mu > 0$ is a consequence of the interlacing property proved in Section 2. It is of interest, however, to produce formulae similar to (3.9), (3.9′) for σ^*_μ. To do so, write $\tau^*_\mu = \cos\theta^*_\mu$ and use [cf. (1.6*)]

$$\gamma = \frac{\cos(n+1)\theta^*_\mu}{\cos(n-1)\theta^*_\mu}, \qquad n \geq 2, \quad \theta^*_\mu \neq \pi/2 \text{ if } n \text{ is even.}$$

Then a computation very similar to the one above for σ_ν, using the known formula (Monegato [4])

$$(3.10) \qquad \sigma^*_\mu = \frac{\|\pi_n\|^2_{d\sigma_\gamma}}{\pi_n(\tau^*_\mu)\pi^{*\prime}_{n+1}(\tau^*_\mu)}, \qquad \mu = 1, 2, \ldots, n+1,$$

in place of (3.2), yields

$$(3.11) \qquad \begin{aligned} \sigma^{*(n)}_\mu &= \frac{\pi}{2}\frac{\cos^2 n\theta^*_\mu}{n + \sin 2n\theta^*_\mu/\sin 2\theta^*_\mu}, \qquad \mu = 1, 2, \ldots, n+1; \\ & \qquad n \geq 2, \quad \mu \neq \frac{n+2}{2} \text{ if } n \text{ is even,} \end{aligned}$$

and

$$(3.11') \qquad \begin{aligned} \sigma_1^{*(1)} = \sigma_2^{*(1)} &= \frac{\pi}{4}\frac{(1+\gamma)^2}{2+\gamma}; \\ \sigma^{*(n)}_{(n+2)/2} &= \frac{\pi}{2}\frac{1+\gamma}{1-\gamma+n(1+\gamma)}, \quad n(\text{even}) \geq 2. \end{aligned}$$

If the points τ_ν in (1.1) are augmented by ± 1, they become the Lobatto points with respect to the measure $d\tilde{\sigma}_\gamma(t) = (1-t^2)^{-1} d\sigma_\gamma(t)$, $-1 < \gamma < 1$, and together with the nodes τ^*_μ, one obtains in

$$(3.12) \quad \int_{-1}^1 f(t)\, d\tilde{\sigma}_\gamma(t) = \tilde{\sigma}_{n+1} f(-1) + \sum_{\nu=1}^n \tilde{\sigma}_\nu f(\tau_\nu) + \tilde{\sigma}_0 f(1) + \sum_{\mu=1}^{n+1} \tilde{\sigma}^*_\mu f(\tau^*_\mu) + \tilde{R}_n(f)$$

the Kronrod extension of the $(n+2)$-point Gauss-Lobatto formula for the measure $d\tilde{\sigma}_\gamma$ (cf. [1, Example 2.3]). Here,

$$(3.13) \quad \tilde{\sigma}_\nu = \frac{\sigma_\nu}{1-\tau_\nu^2}, \qquad \nu = 1, 2, \ldots, n; \qquad \tilde{\sigma}^*_\mu = \frac{\sigma^*_\mu}{1-\tau^{*2}_\mu}, \qquad \mu = 1, 2, \ldots, n+1;$$

and by a formula analogous to (3.2),

$$(3.14) \qquad \begin{aligned} \tilde{\sigma}_0^{(1)} = \tilde{\sigma}_2^{(1)} &= \frac{\pi}{4}\frac{(1+\gamma)^2}{(1-\gamma)(2-\gamma)}, \\ \tilde{\sigma}_0^{(n)} = \tilde{\sigma}_{n+1}^{(n)} &= \frac{\pi}{4}\frac{(1+\gamma)^2}{(1-\gamma)(1+\gamma+n(1-\gamma))}, \qquad n \geq 2. \end{aligned}$$

Hence, all weights in (3.12) are positive for $-1 < \gamma < 1$ and all $n \geq 1$.

We conclude by noting that the Gauss nodes $\tau_\nu^{(n)}$ for the measure (1.5) can be computed most conveniently as eigenvalues of the symmetric tridiagonal $n \times n$-matrix having zeros on the diagonal and the quantities $\sqrt{\beta_1} = \frac{1}{2}\sqrt{1+\gamma}$, $\sqrt{\beta_2} = \cdots = \sqrt{\beta_{n-1}} = \frac{1}{2}$ on the two side diagonals, if $n \geq 2$. (If $n = 1$ then $\tau_1^{(1)} = 0$.) Likewise, $\tau_\mu^{*(n)}$, $n \geq 1$, are computable as eigenvalues of the symmetric tridiagonal $(n+1) \times (n+1)$-matrix with zero diagonal and $\sqrt{\beta_1^*} = \sqrt{\frac{1}{2}(1+\gamma)}$, $\sqrt{\beta_2^*} = \frac{1}{2}\sqrt{1-\gamma}, \sqrt{\beta_3^*} = \cdots = \sqrt{\beta_n^*} = \frac{1}{2}$ on the side diagonals, if $n \geq 2$, and $\sqrt{\beta_1^*} = \frac{1}{2}\sqrt{2+\gamma}$ on the side diagonals, if $n = 1$.

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1. W. GAUTSCHI, "Gauss-Kronrod quadrature–A survey," in *Numerical Methods and Approximation Theory III* (G. V. Milovanović, ed.), University of Niš, Niš, 1988, pp. 39–66.

2. W. GAUTSCHI & S. E. NOTARIS, "An algebraic study of Gauss-Kronrod quadrature formulae for Jacobi weight functions," *Math. Comp.*, v. 51, 1988, pp. 231–248.

3. J. GERONIMUS, "On a set of polynomials," *Ann. of Math.*, v. 31, 1930, pp. 681–686.

4. G. MONEGATO, "A note on extended Gaussian quadrature rules," *Math. Comp.*, v. 30, 1976, pp. 812–817.

5. G. MONEGATO, "Positivity of the weights of extended Gauss-Legendre quadrature rules," *Math. Comp.*, v. 32, 1978, pp. 243–245.

6. G. MONEGATO, "Stieltjes polynomials and related quadrature rules," *SIAM Rev.*, v. 24, 1982, pp. 137–158.

7. G. SZEGÖ, "Über gewisse orthogonale Polynome, die zu einer oszillierenden Belegungsfunktion gehören," *Math. Ann.*, v. 110, 1935, pp. 501–513. [*Collected Papers* (R. Askey, ed.), v. 2, pp. 545–557.]

8. G. SZEGÖ, *Orthogonal Polynomials*, Amer. Math. Soc. Colloq. Publ., vol. 23, 4th ed., Amer. Math. Soc., Providence, R. I., 1975.