

INTERNALITY OF TWO-MEASURE-BASED GENERALIZED GAUSS QUADRATURE RULES FOR MODIFIED CHEBYSHEV MEASURES*

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Dedicated to our friend Giuseppe Rodriguez on the occasion of his 60th birthday.

Abstract. Many applications in science and engineering require the approximation of integrals of the form $\int_{-1}^1 f(x)d\sigma(x)$, where f is an integrand and $d\sigma$ is a nonnegative measure. Such approximations often are computed by an ℓ -node Gauss quadrature rule $G_\ell(f)$ that is determined by the measure. It is important to be able to estimate the quadrature error in these approximations. Error estimates can be computed by applying another quadrature rule, $Q_m(f)$, with $m > \ell$ nodes, and using the difference $Q_m(f) - G_\ell(f)$ as an estimate for the error in $G_\ell(f)$. This paper considers the situation when $d\sigma$ is a modified Chebyshev measure and shows that two-measure-based quadrature rules $\widehat{Q}_{2\ell+1}$ exist, have positive weights, and have distinct nodes in the interval $[-1, 1]$. The last property makes them applicable also when the integrand f only is defined in $[-1, 1]$. Comparisons with other choices of quadrature formulas $Q_{2\ell+1}$ are presented. This paper extends the investigation of two-measure-based quadrature rules for Jacobi and generalized Laguerre measures initiated in A. V. Pejčev et. al [Appl. Numer. Math., 204 (2024), pp. 206–221].

Key words. Gauss quadrature rule, averaged Gauss rule, generalized averaged Gauss rule, modified Chebyshev measure

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1. Introduction. Let $d\sigma$ be a Chebyshev measure that is modified by a linear divisor and a linear factor, i.e., we consider measures of the form

$$(1.1) \quad d\sigma(x) = d\sigma_1(x) = \frac{x - \gamma}{x - \delta} \frac{1}{\sqrt{1 - x^2}} dx \quad \text{for } -1 < x < 1,$$

$$(1.2) \quad d\sigma(x) = d\sigma_2(x) = \frac{x - \gamma}{x - \delta} \sqrt{1 - x^2} dx \quad \text{for } -1 < x < 1,$$

$$(1.3) \quad d\sigma(x) = d\sigma_3(x) = \frac{x - \gamma}{x - \delta} \sqrt{\frac{1+x}{1-x}} dx \quad \text{for } -1 < x < 1,$$

where

$$(1.4) \quad \gamma = -\left(\frac{1}{2}c + c^{-1}\right), \quad \delta = -\frac{1}{2}(c + c^{-1}),$$

and $c \in \mathbb{R} \setminus \{0\}$ in the cases (1.1) and (1.2), while $c \in \mathbb{R} \setminus \{-1, 0\}$ in the case (1.3) (cf. [5]), since the zeroth moment cannot be calculated in the case $c = -1$. Thus, the measure $d\sigma_i(x)$

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is a modification of the Chebyshev measure of the i -th kind for $i \in \{1, 2, 3\}$. Quadrature rules and orthogonal polynomials for modified Chebyshev measures have previously been discussed by Djukić et al. [3, 4, 5, 6, 10] and Milovanović et al. [14]

We are concerned with the approximation of integrals of the form

$$(1.5) \quad I(f) = \int_{-1}^1 f(x) d\sigma(x)$$

for some integrand f by an ℓ -node interpolatory quadrature formula

$$Q_\ell(f) = \sum_{j=1}^{\ell} \omega_j f(x_j)$$

with real distinct nodes x_j and real weights ω_j . Let the quadrature error

$$R_\ell(f) = I(f) - Q_\ell(f)$$

satisfy $R_\ell(f) = 0$, for $f \in \mathcal{P}_{2\ell-m-1}$, for some $0 \leq m \leq \ell$, where \mathcal{P}_j denotes the set of polynomials of degree at most j . We then refer to Q_ℓ as a $(2\ell - m - 1, \ell, d\sigma)$ -quadrature formula. If, in addition, all weights ω_j are positive, then Q_ℓ is referred to as a *positive* $(2\ell - m - 1, n, d\sigma)$ -quadrature formula. We say that a polynomial

$$(1.6) \quad t_\ell(x) = \prod_{j=1}^{\ell} (x - x_j)$$

generates a $(2\ell - m - 1, \ell, d\sigma)$ -quadrature formula if t_ℓ has ℓ simple zeros x_j and if the interpolatory quadrature formula based on the nodes x_j is a $(2\ell - m - 1, \ell, d\sigma)$ -quadrature formula. A $(2\ell - m - 1, \ell, d\sigma)$ -quadrature formula is said to be *internal* if all its nodes belong to the interval $[-1, 1]$. A node outside this interval is said to be *external*.

The unique interpolatory quadrature formula with ℓ nodes and $m = 0$, i. e., the $(2\ell - 1, \ell, d\sigma)$ -quadrature formula, is the Gauss formula with respect to the measure $d\sigma$,

$$(1.7) \quad G_\ell(f) = \sum_{j=1}^{\ell} \omega_j^G f(x_j^G).$$

This rule has maximal degree of precision, $2\ell - 1$, over all ℓ -node rules, i. e., $I(f) = G_\ell(f)$ for all $f \in \mathcal{P}_{2\ell-1}$. Due to this property and the fact that all nodes live in the open interval $(-1, 1)$, Gauss quadrature formulas are powerful general purpose quadrature rules for the approximation of integrals (1.5).

It is important to be able to estimate the quadrature error

$$(1.8) \quad R_\ell(f) = I(f) - G_\ell(f),$$

or its magnitude, of the Gauss rule (1.7) to determine a suitable number of nodes ℓ . A Gauss rule with too few nodes results in a quadrature error that is larger than desired, while a Gauss rule with unnecessarily many nodes requires the evaluation of the integrand at needlessly many nodes.

The classical approach to estimate the error (1.8) is to compute the $(2\ell + 1)$ -node Gauss-Kronrod rule, $H_{2\ell+1}(f)$, associated with $G_\ell(f)$ and approximate the quadrature error by

the difference $H_{2\ell+1}(f) - G_\ell(f)$. However, Gauss–Kronrod rules do not exist or have real nodes for various measures $d\sigma$ and numbers of nodes ℓ ; see Gautschi [11] or Notaris [15] for the definition of and discussions on Gauss–Kronrod rules. This shortcoming of Gauss–Kronrod rules lead Laurie [13] and M. M. Spalević [19] to develop $(2\ell + 1)$ -node averaged and generalized averaged quadrature rules, which we denote by $\tilde{G}_{2\ell+1}$ and $\hat{G}_{2\ell+1}$, respectively, for the estimation of the error in G_ℓ similarly as the Gauss–Kronrod rule $H_{2\ell+1}$. These rules have $2\ell + 1$ nodes, ℓ of which agree with the nodes of the Gauss rule G_ℓ , and they exist when the Gauss rule G_ℓ exists.

However, averaged and generalized averaged rules are not internal for certain measures, among them the measures (1.1) and (1.3); see [3, 4, 5, 6, 8, 9, 10] for analyses. They therefore cannot be applied for these measures when the integrand f is defined on the interval $[-1, 1]$ only. A few ways to circumvent this difficulty are described in [6, 7, 18]. Here we analyze an approach that recently was proposed in [17] for estimating the error in G_ℓ . It is based on constructing a $(2\ell + 1)$ -node quadrature formula using the measure $d\sigma$ as well as an auxiliary measure $d\mu$ also with support in the interval $[-1, 1]$. We refer to these quadrature rules as *two-measure-based generalized Gauss quadrature formulas*. They are referred to as *new averaged Gauss (NAG) quadrature formulas* in [17]. We also will use this acronym below, and we denote these rules by $\hat{Q}_{2\ell+1}$. Their application to the estimation of the error in G_ℓ is particularly attractive when the rule $\hat{Q}_{2\ell+1}$ is internal, but the rules $\tilde{G}_{2\ell+1}$, $\hat{G}_{2\ell+1}$, and $H_{2\ell+1}$ are not. The quadrature formulas $\hat{Q}_{2\ell+1}$ are easy to compute; this is discussed in Section 2. Their nodes generally are distinct from the nodes of G_ℓ . This is not a major concern when it is inexpensive to evaluate the integrand f at the quadrature nodes. The rule $\hat{Q}_{2\ell+1}$ has the same degree of precision as the generalized averaged Gauss quadrature rule $\hat{G}_{2\ell+1}$, i.e., at least $2\ell + 2$; see [17]. Typically, the degree of precision of the rule $\hat{G}_{2\ell+1}$ is higher than that of the averaged Gauss quadrature rule $\tilde{G}_{2\ell+1}$, whose degree of precision is at least $2\ell + 1$; see [13].

This paper is organized as follows. Section 2 describes the NAG rules $\hat{Q}_{2\ell+1}$, and Sections 3–5 discuss, analyze, and illustrate the performance of these rules associated with modified Chebyshev measures of the first, second, and third kinds. Concluding remarks can be found in Section 6.

We conclude this section by noting that similar results to the ones for NAG rules $\hat{Q}_{2\ell+1}$ associated with a modified Chebyshev measure of the third kind also hold for analogous quadrature rules associated with a modified Chebyshev measure of the fourth kind

$$d\sigma(x) = d\sigma_4(x) = \frac{x - \gamma}{x - \delta} \sqrt{\frac{1-x}{1+x}} dx \quad \text{for } -1 < x < 1,$$

which are obtained by replacing c by $-c$ in (1.4); see the comment just above Section 4 in [5].

2. NAG quadrature formulas. Let p_k denote the monic polynomial of degree k that is orthogonal to \mathcal{P}_{k-1} with respect to the measure $d\sigma$, i.e.,

$$\int_a^b x^j p_k(x) d\sigma(x) = 0, \quad j = 0, 1, \dots, k-1.$$

It is well known that the polynomials p_k , $k = 0, 1, \dots$, satisfy a three-term recurrence relation of the form

$$p_{k+1}(x) = (x - \alpha_k)p_k(x) - \beta_k p_{k-1}(x), \quad k = 0, 1, \dots,$$

where $p_{-1}(x) \equiv 0$, $p_0(x) \equiv 1$, $\alpha_k \in \mathbb{R}$, and $\beta_k > 0$ for all k ; see, e. g., Gautschi [11] for details. The zeros of the polynomial p_ℓ are the nodes of the Gauss rule (1.7). They also are the

averaged rule $\tilde{G}_{2\ell+1}$ for the measure (1.1) is external, and in [3, Theorem 7] that both extreme nodes of the generalized averaged Gauss formula $\hat{G}_{2\ell+1}$ for this measure are external. We are interested in deriving NAG quadrature rules $\hat{Q}_{2\ell+1}$ that are internal.

We obtain from [3] that the monic orthogonal polynomials associated with the measure $d\sigma_1(x)$ are given by

$$(3.1) \quad \hat{P}_k(x) = \frac{\tilde{P}_{k+1}(x) - r_k \tilde{P}_k(x)}{x - \gamma}, \quad \text{where} \quad r_k = \frac{\tilde{P}_{k+1}(\gamma)}{\tilde{P}_k(\gamma)},$$

under the assumption that $\tilde{P}_k(\gamma) \neq 0$ for all k ; see [3, Eq. (13)]. Here the \tilde{P}_k are the monic polynomials

$$\tilde{P}_k(x) = \frac{1}{2^{k-1}} (T_k(x) + \acute{c} T_{k-1}(x)) \quad \text{for } k \geq 2,$$

with $\tilde{P}_0(x) = 1$ and $\tilde{P}_1(x) = x + \acute{c}$. The constant \acute{c} is defined by

$$\acute{c} = \min\{c, c^{-1}\},$$

and the T_k are Chebyshev polynomials of the first kind scaled so that

$$T_k(\cos \xi) = \cos k\xi.$$

Hence, $T_k(\pm 1) = (\pm 1)^k$. The corresponding monic Chebyshev polynomials $\overset{\circ}{T}_k$ satisfy

$$\overset{\circ}{T}_k(\pm 1) = \frac{(\pm 1)^k}{2^{k-1}};$$

see [3] for a detailed derivation of the polynomials (3.1).

In view of (1.4), the parameter $\gamma = \gamma(c)$ satisfies

$$(3.2) \quad \gamma'(c) = \frac{2 - c^2}{2c^2},$$

and, therefore, $\gamma'(c) = 0$ for $c = \sqrt{2}$. Hence, $\gamma_{\max} = \gamma(\sqrt{2}) = -\sqrt{2}$, i. e., $\gamma \leq -\sqrt{2}$ and $x - \gamma \geq x + \sqrt{2} \geq -1 + \sqrt{2} > 0$.

Consider the NAG quadrature rule $\hat{Q}_{2\ell+1}$ that corresponds to the Jacobi matrix (2.5). This rule is of the form $(2\ell + 2, 2\ell + 1, d\sigma, d\mu)$, where $d\mu$ is defined by (2.4). The monic orthogonal polynomial $\overset{\circ}{U}_k$ of degree k associated with this measure satisfies

$$\overset{\circ}{U}_k(\pm 1) = \frac{k+1}{2^k} (\pm 1)^k;$$

see, e.g., [11, p. 28].

The (monic) polynomial $t_{2\ell+1}$ in (2.3) associated with the rule $\hat{Q}_{2\ell+1}$ is of the form

$$t_{2\ell+1}(x) = \hat{P}_{\ell+1}(x) \overset{\circ}{U}_\ell(x) - \hat{\beta}_{\ell+1} \hat{P}_\ell(x) \overset{\circ}{U}_{\ell-1}(x),$$

which we express as

$$(3.3) \quad t_{2\ell+1}(x) = \frac{\tilde{P}_{\ell+2}(x) - r_{\ell+1} \tilde{P}_{\ell+1}(x)}{x - \gamma} \overset{\circ}{U}_\ell(x) - \hat{\beta}_{\ell+1} \frac{\tilde{P}_{\ell+1}(x) - r_\ell \tilde{P}_\ell(x)}{x - \gamma} \overset{\circ}{U}_{\ell-1}(x),$$

where (cf. [3, Eq. 15])

$$(3.4) \quad \widehat{\beta}_\ell = \frac{r_\ell}{4r_{\ell-1}} \quad (\ell \geq 2)$$

and

$$(3.5) \quad r_\ell = -\frac{1}{2} \frac{z^{\ell-1} - Az^{1-\ell}}{z^{\ell-2} - Az^{2-\ell}}$$

with (cf. [3, Eq. 18])

$$A = \frac{1 + 2z^{-1}r_1}{1 + 2zr_1}$$

and (cf. [3, Eq. 16])

$$(3.6) \quad z = \frac{c^2 + 2 + \sqrt{c^4 + 4}}{2c}.$$

Note that

$$z^{-1} = \frac{c^2 + 2 - \sqrt{c^4 + 4}}{2c}.$$

Therefore, $z = z(c)$ satisfies $z \geq \sqrt{2} + 1$ with equality for $c = \sqrt{2}$. The inequalities

$$(3.7) \quad 0 < A < z^{-2} < 1,$$

shown in [3, Eq. 20], will be used below.

The largest node of the quadrature rule $\widehat{Q}_{2\ell+1}$ is smaller than or equal to 1 if $t_{2\ell+1}(1) \geq 0$ holds. In view of (3.3), this is equivalent to

$$\frac{\widetilde{P}_{\ell+2}(1) - r_{\ell+1}\widetilde{P}_{\ell+1}(1)}{1 - \gamma} \overset{\circ}{U}_\ell(1) - \widehat{\beta}_{\ell+1} \frac{\widetilde{P}_{\ell+1}(1) - r_\ell\widetilde{P}_\ell(1)}{1 - \gamma} \overset{\circ}{U}_{\ell-1}(1) \geq 0,$$

i.e.,

$$\begin{aligned} & \frac{\frac{1}{2^{\ell+1}}(T_{\ell+2}(1) + \acute{c}T_{\ell+1}(1)) - r_{\ell+1}\frac{1}{2^\ell}(T_{\ell+1}(1) + \acute{c}T_\ell(1))}{1 - \gamma} \overset{\circ}{U}_\ell(1) \\ & - \widehat{\beta}_{\ell+1} \frac{\frac{1}{2^\ell}(T_{\ell+1}(1) + \acute{c}T_\ell(1)) - r_\ell\frac{1}{2^{\ell-1}}(T_\ell(1) + \acute{c}T_{\ell-1}(1))}{1 - \gamma} \overset{\circ}{U}_{\ell-1}(1) \geq 0. \end{aligned}$$

Substituting the expressions for $T_\ell(1)$ and $\overset{\circ}{U}_\ell(1)$ provided above into this inequality yields

$$\begin{aligned} & \frac{\frac{1}{2^{\ell+1}}(1 + \acute{c}) - r_{\ell+1}\frac{1}{2^\ell}(1 + \acute{c})}{1 - \gamma} \frac{\ell + 1}{2^\ell} \\ & - \widehat{\beta}_{\ell+1} \frac{\frac{1}{2^\ell}(1 + \acute{c}) - r_\ell\frac{1}{2^{\ell-1}}(1 + \acute{c})}{1 - \gamma} \frac{\ell}{2^{\ell-1}} \geq 0. \end{aligned}$$

Multiplying this inequality by $2 \cdot 4^\ell \cdot (1 - \gamma)/(1 + \acute{c})$ gives

$$(1 - 2r_{\ell+1})(\ell + 1) - 4\widehat{\beta}_{\ell+1}\ell(1 - 2r_\ell) \geq 0$$

and using (3.4), we obtain

$$\frac{1 - 2r_{\ell+1}}{1 - 2r_\ell} \geq \frac{\ell}{\ell + 1} \frac{r_{\ell+1}}{r_\ell}.$$

Application of (3.5) now yields

$$\frac{1 - 2(-\frac{1}{2}) \frac{z^\ell - Az^{-\ell}}{z^{\ell-1} - Az^{1-\ell}}}{1 - 2(-\frac{1}{2}) \frac{z^{\ell-1} - Az^{1-\ell}}{z^{\ell-2} - Az^{2-\ell}}} \geq \frac{\ell}{\ell + 1} \frac{-\frac{1}{2} \frac{z^\ell - Az^{-\ell}}{z^{\ell-1} - Az^{1-\ell}}}{-\frac{1}{2} \frac{z^{\ell-1} - Az^{1-\ell}}{z^{\ell-2} - Az^{2-\ell}}}.$$

This expression simplifies to

$$\frac{z^{\ell-1} - Az^{-\ell}}{z^{\ell-2} - Az^{1-\ell}} \geq \frac{\ell}{\ell + 1} \frac{z^\ell - Az^{-\ell}}{z^{\ell-1} - Az^{1-\ell}},$$

which gives

$$\begin{aligned} & (\ell + 1) (z^{2\ell-2} - A - Az^{-1} + A^2 + A^2 z^{-2\ell+1}) \\ & \geq \ell (z^{2\ell-2} - Az^{-2} - Az + A^2 + A^2 z^{-2\ell+1}). \end{aligned}$$

This reduces to

$$z^{2\ell-2} + \ell A(1 - z)(z^{-2} - 1) + A^2 z^{-2\ell+1} \geq A(1 + z^{-1}).$$

The last inequality holds for $\ell \geq 2$ since in view of $z \geq \sqrt{2} + 1$ and (3.7), we have

$$\ell A(1 - z)(z^{-2} - 1) > 0, \quad A^2 z^{-2\ell+1} > 0,$$

and

$$z^{2\ell-2} \geq (1 + \sqrt{2})^{2\ell-2} \geq (1 + \sqrt{2})^2 = 3 + 2\sqrt{2} > A(1 + z^{-1}) \in (0, 2).$$

We turn to the smallest node of the NAG quadrature rule $\widehat{Q}_{2\ell+1}$. It will be larger than or equal to -1 if $t_{2\ell+1}(-1) \leq 0$ holds. Proceeding similarly as above, this is equivalent to

$$\begin{aligned} & \frac{(-1)^{\ell+2} \frac{1}{2^{\ell+1}} (1 - \hat{c}) - r_{\ell+1} (-1)^{\ell+1} \frac{1}{2^\ell} (1 - \hat{c})}{-1 - \gamma} (-1)^\ell \frac{\ell + 1}{2^\ell} \\ & - \widehat{\beta}_{\ell+1} \frac{(-1)^{\ell+1} \frac{1}{2^\ell} (1 - \hat{c}) - r_\ell (-1)^\ell \frac{1}{2^{\ell-1}} (1 - \hat{c})}{-1 - \gamma} (-1)^{\ell-1} \frac{\ell}{2^{\ell-1}} \leq 0. \end{aligned}$$

Multiplying this inequality by $2 \cdot 4^\ell \cdot (-1 - \gamma)/(1 - \hat{c})$, we get

$$(1 + 2r_{\ell+1})(\ell + 1) - 4\widehat{\beta}_{\ell+1}\ell(1 + 2r_\ell) \leq 0.$$

Using (3.4) gives

$$(3.8) \quad \frac{1 + 2r_{\ell+1}}{1 + 2r_\ell} \geq \frac{\ell}{\ell + 1} \frac{r_{\ell+1}}{r_\ell},$$

since (see (3.5))

$$\begin{aligned} 1 + 2r_\ell &= 1 + 2 \left(-\frac{1}{2} \right) \frac{z^{\ell-1} - Az^{1-\ell}}{z^{\ell-2} - Az^{2-\ell}} \\ &= \frac{(1 - z)(z^{\ell-2} + Az^{1-\ell})}{z^{\ell-2} - Az^{2-\ell}} < 0. \end{aligned}$$

The inequality (3.8) can be expressed as

$$\frac{1 + 2 \left(-\frac{1}{2} \right) \frac{z^\ell - Az^{-\ell}}{z^{\ell-1} - Az^{1-\ell}}}{1 + 2 \left(-\frac{1}{2} \right) \frac{z^{\ell-1} - Az^{1-\ell}}{z^{\ell-2} - Az^{2-\ell}}} \geq \frac{\ell}{\ell + 1} \frac{-\frac{1}{2} \frac{z^\ell - Az^{-\ell}}{z^{\ell-1} - Az^{1-\ell}}}{-\frac{1}{2} \frac{z^{\ell-1} - Az^{1-\ell}}{z^{\ell-2} - Az^{2-\ell}}}.$$

Some simplifications yield

$$\frac{z^{\ell-1} + Az^{-\ell}}{z^{\ell-2} + Az^{1-\ell}} \geq \frac{\ell}{\ell + 1} \frac{z^\ell - Az^{-\ell}}{z^{\ell-1} - Az^{1-\ell}},$$

i.e.,

$$\begin{aligned} & (\ell + 1) (z^{2\ell-2} - A + Az^{-1} - A^2 z^{-2\ell+1}) \\ & \geq \ell (z^{2\ell-2} - Az^{-2} + Az - A^2 z^{-2\ell+1}), \end{aligned}$$

which reduces to

$$z^{2\ell-2} + \ell A(1+z)(1-z^{-2}) \geq A(1-z^{-1}) + A^2 z^{-2\ell+1}.$$

The last inequality holds for $\ell \geq 2$, because due to $z \geq \sqrt{2} + 1$ and (3.7), we have

$$\ell A(1+z)(1-z^{-2}) > 0$$

and

$$z^{2\ell-2} \geq 3 + 2\sqrt{2} > A(1-z^{-1}) + A^2 z^{-2\ell+1} \in (0, 2).$$

We have shown the following result.

THEOREM 3.1. *The NAG quadrature rule $\widehat{Q}_{2\ell+1}$ of the form $(2\ell + 2, 2\ell + 1, d\sigma_1, d\mu)$, where $d\mu$ is defined by (2.4), is internal, i.e., all its nodes are in the interval $[-1, 1]$, for every $\ell \geq 2$.*

3.1. A numerical example for the measure $d\sigma_1(x)$. Computed examples in which the quadrature error in Gauss rules G_ℓ , for several values of ℓ and of the parameter $c > 0$, are estimated by averaged Gauss quadrature rules $\widehat{G}_{2\ell+1}$, generalized averaged Gauss rules $\widehat{G}_{2\ell+1}$, and truncated generalized averaged Gauss rules $Q_{\ell+2}^{(1)}$ are presented in [3]. We complement these results with error estimation with the NAG quadrature rules $\widehat{Q}_{2\ell+1}$.

Consider the integral

$$I(f) = \int_{-1}^1 f(x) d\sigma_1(x)$$

with the integrand

$$f(x) = 999.1^{\log_{10}(1+\varepsilon+x)}, \quad \text{where } \varepsilon = 10^{-6}.$$

This integrand has a singularity at $x = -1 - \varepsilon$, very close to the support of the measure. Since the rules $\widetilde{G}_{2\ell+1}$ and $\widehat{G}_{2\ell+1}$ have a node smaller than $-1 - \varepsilon$, they cannot be used. However, the truncated rule $Q_{\ell+2}^{(1)}$ is internal and provides error estimates of the correct order

of magnitude. We tabulate the magnitude of these estimates and of those determined with the NAG rule $\widehat{Q}_{2\ell+1}(f)$, which according to Theorem 3.1 is internal. Table 3.1 displays

$$E_{TGA} = \left| Q_{\ell+2}^{(1)}(f) - G_{\ell}(f) \right|,$$

$$E_{NAG} = \left| \widehat{Q}_{2\ell+1}(f) - G_{\ell}(f) \right|,$$

for some values of ℓ and $c > 0$. The entries of the column with the header “Error” display the magnitude of the actual quadrature errors, which are computed with high-precision arithmetic. All quadrature rules and table entries of this paper are computed with about 20 significant decimal digits.

Observe that the error estimates E_{NAG} are closer to the actual quadrature error for $G_{\ell}(f)$ than the corresponding error estimates E_{TGA} . The exact value of the integral is $I(f) \approx 11.9094$ for $c = 0.5$, and $I(f) \approx 8.8666$ for $c = 2$. These values help us assess the relative quadrature errors in magnitude.

TABLE 3.1
The error estimates E_{TGA} , E_{NAG} , and the actual error in the column labeled “Error”.

c	ℓ	E_{TGA}	E_{NAG}	Error
0.5	5	6.8789(−8)	7.5822(−8)	7.6155(−8)
	10	4.5475(−10)	6.3428(−10)	6.3826(−10)
	15	2.2961(−11)	3.9631(−11)	3.9905(−11)
	20	2.6705(−12)	5.5240(−12)	5.5638(−12)
	30	1.2312(−13)	3.4049(−13)	3.4303(−13)
2	5	3.5371(−8)	3.8815(−8)	3.8968(−8)
	10	2.1419(−10)	2.9654(−10)	2.9828(−10)
	15	1.0378(−11)	1.7776(−11)	1.7892(−11)
	20	1.1779(−12)	2.4191(−12)	2.4358(−12)
	30	5.2821(−14)	1.4520(−13)	1.4625(−13)

We conclude with some comments on the computational effort required to evaluate the quadrature rules $\widehat{Q}_{2\ell+1}$ and $Q_{\ell+2}^{(1)}$. The evaluation of the nodes and weights of both rules requires $\mathcal{O}(\ell^2)$ flops by using the Golub–Welsch algorithm or a divide-and-conquer method, with the flop count for the rule $Q_{\ell+2}^{(1)}$ being somewhat smaller since this rule only has $\ell + 2$ nodes. Given the nodes and weights for these rules, the computation of the value $Q_{\ell+2}^{(1)}(f)$ is cheaper than the calculation of $\widehat{Q}_{2\ell+1}(f)$ since the former rule only requires the evaluations of the function f at $\ell + 2$ nodes, while the latter rule demands the evaluation of f at $2\ell + 1$ nodes. For most quadrature problems, the difference in the computational effort is insignificant, and the higher accuracy of the error estimates delivered by the rules $\widehat{Q}_{2\ell+1}$ makes their application attractive.

4. Internality of NAG quadrature rules $\widehat{Q}_{2\ell+1}$ determined by modified Chebyshev measures of the second kind. Since the generalized averaged Gauss quadrature rules $\widehat{G}_{2\ell+1}$ are internal for modified Chebyshev measures of the second kind (1.2) (see [10]), there is no need to use NAG rules $\widehat{Q}_{2\ell+1}$. We therefore omit their analysis.

5. Internality of NAG quadrature rules $\widehat{Q}_{2\ell+1}$ determined by modified Chebyshev measures of the third kind. We are concerned with the integration of integrals (1.5) with the measure $d\sigma$ given by (1.3) and will use NAG quadrature rules $(2\ell + 2, 2\ell + 1, d\sigma_3, d\mu)$ that are determined by the measures (1.3) and (2.4). Our analysis uses results and notation from [5].

Let γ in (1.3) be defined by (1.4) for some $c \in \mathbb{R} \setminus \{0\}$. It is shown in [5, Theorem 5] that the generalized averaged quadrature rule $\widehat{G}_{2\ell+1}$ is not internal when $c < 0$, specifically its largest node is larger than 1. Moreover, [5, Theorem 5] shows that for any real nonvanishing parameter c , the averaged Gauss quadrature rule $\widetilde{G}_{2\ell+1}$ is not internal. It is therefore of interest to determine NAG quadrature rules $\widehat{Q}_{2\ell+1}$ that are internal.

Let γ be defined as describe above and introduce

$$(5.1) \quad \acute{c} = \begin{cases} c, & |c| < 1, \\ c^{-1}, & |c| \geq 1. \end{cases}$$

Consider Chebyshev polynomials of the third kind of degree k ,

$$V_k(\cos \xi) = \frac{\cos(k + \frac{1}{2})\xi}{\cos \frac{\xi}{2}}, \quad k = 0, 1, 2, \dots$$

Then $V_k(1) = 1$ and $V_k(-1) = (2k + 1)(-1)^k$. Define the monic polynomials

$$\widetilde{P}_k(x) = \frac{1}{2^k} (V_k(x) + \acute{c}V_{k-1}(x)) \quad \text{for } k \geq 1,$$

with $\widetilde{P}_0(x) = 1$ and $\widetilde{P}_1(x) = x + \acute{c}$, where \acute{c} is given by (5.1). Then the monic orthogonal polynomials \widehat{P}_k , $k = 0, 1, 2, \dots$, with respect to the measure (1.3) are given by (3.1) provided that $\widetilde{P}_k(\gamma) \neq 0$ for all k ; see [5] for details. It follows from (3.2) that for $c < 0$ it holds that $\gamma_{\min} = \gamma(-\sqrt{2}) = \sqrt{2}$, i.e., $\gamma \geq \sqrt{2}$. The monic polynomial $t_{2\ell+1}$ in (2.3) has the form (3.3), where (cf. [5, Eq. 18])

$$(5.2) \quad \widehat{\alpha}_\ell = r_{\ell+1} - r_\ell - 1, \quad \widehat{\beta}_\ell = \frac{r_\ell}{4r_{\ell-1}} \quad (\ell \geq 2)$$

and

$$(5.3) \quad r_\ell = -\frac{1}{2z} \frac{z^{2\ell-2} + A}{z^{2\ell-4} + A} \quad (\ell \in \mathbb{N}).$$

By [5, Eq. 21],

$$A = \begin{cases} z^{-5} \left(\frac{c^2 + \sqrt{c^4 + 4}}{2} \right)^2, & |c| < 1, \\ z^{-3} \left(\frac{c^2 + \sqrt{c^4 + 4}}{2} \right)^{-2}, & |c| \geq 1, \end{cases}$$

where z is given by (3.6). It can easily be seen that $z \leq -\sqrt{2} - 1$, with equality for $c = -\sqrt{2}$, if $c < 0$. Further, $z \geq 1 + \sqrt{2}$, with equality for $c = \sqrt{2}$, if $c > 0$. In either case, A has the same sign as z and c . Moreover,

$$(5.4) \quad 0 < |A| < |z|^{-3};$$

see [5, Eq. 22].

The largest node of the rule $\widehat{Q}_{2\ell+1}$ is smaller than or equal to 1 if $t_{2\ell+1}(1) \geq 0$. In view of (3.3), this can be expressed as

$$\begin{aligned} & \frac{\frac{1}{2^{\ell+2}} (V_{\ell+2}(1) + \acute{c} V_{\ell+1}(1)) - r_{\ell+1} \frac{1}{2^{\ell+1}} (V_{\ell+1}(1) + \acute{c} V_{\ell}(1))}{1 - \gamma} \overset{\circ}{U}_{\ell}(1) \\ & - \widehat{\beta}_{\ell+1} \frac{\frac{1}{2^{\ell+1}} (V_{\ell+1}(1) + \acute{c} V_{\ell}(1)) - r_{\ell} \frac{1}{2^{\ell}} (V_{\ell}(1) + \acute{c} V_{\ell-1}(1))}{1 - \gamma} \overset{\circ}{U}_{\ell-1}(1) \geq 0. \end{aligned}$$

Using the explicitly known values of $V_{\ell}(1)$ and $\overset{\circ}{U}_{\ell}(1)$, this inequality can be written as

$$\begin{aligned} & \frac{\frac{1}{2^{\ell+2}} (1 + \acute{c}) - r_{\ell+1} \frac{1}{2^{\ell+1}} (1 + \acute{c})}{1 - \gamma} \frac{\ell + 1}{2^{\ell}} \\ & - \widehat{\beta}_{\ell+1} \frac{\frac{1}{2^{\ell+1}} (1 + \acute{c}) - r_{\ell} \frac{1}{2^{\ell}} (1 + \acute{c})}{1 - \gamma} \frac{\ell}{2^{\ell-1}} \geq 0. \end{aligned}$$

Multiplication by $4^{\ell+1}(1 - \gamma)/(1 + \acute{c})$ gives the expression

$$(1 - 2r_{\ell+1})(\ell + 1) - 4\widehat{\beta}_{\ell+1}\ell(1 - 2r_{\ell}) \leq 0,$$

where we have used that $1 + \acute{c} > 0$ and $1 - \gamma < 0$. Using (5.2), we obtain the inequality

$$\frac{1 - 2r_{\ell+1}}{1 - 2r_{\ell}} \leq \frac{\ell}{\ell + 1} \frac{r_{\ell+1}}{r_{\ell}},$$

and substituting (5.3) into this expression gives

$$\frac{1 - 2(-\frac{1}{2z}) \frac{z^{2\ell} + A}{z^{2\ell-2} + A}}{1 - 2(-\frac{1}{2z}) \frac{z^{2\ell-2} + A}{z^{2\ell-4} + A}} \leq \frac{\ell}{\ell + 1} \frac{-\frac{1}{2z} \frac{z^{2\ell} + A}{z^{2\ell-2} + A}}{-\frac{1}{2z} \frac{z^{2\ell-2} + A}{z^{2\ell-4} + A}}.$$

Some simplification yields

$$(\ell + 1)(z^{2\ell-1} + A)(z^{2\ell-2} + A) - \ell(z^{2\ell} + A)(z^{2\ell-3} + A) \leq 0,$$

where we have used that $1 + z < 0$, $z < 0$, and $z^{2\ell-2} > 0$ for $\ell \geq 2$.

After division by $z^{2\ell} (> 0)$, this inequality reduces to

$$(5.5) \quad z^{2\ell-3} + (\ell + 1)Az^{-1}(1 + z^{-1}) - \ell A(1 + z^{-3}) + A^2 z^{-2\ell} \leq 0.$$

To show (5.5) for $\ell \geq 2$, we first observe that due to $-z (\geq \sqrt{2} + 1) > 2$ ($c < 0$) and (5.4), we have

$$z^{-1} \in \left(-\frac{1}{2}, 0\right), \quad 1 + z^{-1} \in (0, 1),$$

$$A \in \left(-\frac{1}{8}, 0\right), \quad Az^{-1} \in \left(0, \frac{1}{16}\right), \quad \ell Az^{-1}(1 + z^{-1}) < \frac{\ell}{16},$$

$$z^{-3} \in \left(-\frac{1}{8}, 0\right), \quad 1 + z^{-3} \in (0, 1), \quad -\ell A(1 + z^{-3}) < \frac{1}{8}\ell,$$

$$A^2 < \frac{1}{64}, \quad z^{-2\ell} < \frac{1}{4^\ell} < \frac{1}{16}, \quad \text{for } \ell \geq 2, \quad A^2 z^{-2\ell} < \frac{1}{16} \cdot \frac{1}{64} = \frac{1}{1024}.$$

Now, inequality (5.5) holds if (for $\ell \geq 2$)

$$z^{2\ell-3} + \frac{\ell+1}{16} + \frac{\ell}{8} + \frac{1}{1024} \leq 0,$$

i.e.,

$$1024z^{2\ell-3} + 192\ell + 65 \leq 0,$$

i.e.,

$$(5.6) \quad 1024a^{2\ell-3} - 192\ell - 65 \geq 0,$$

where $a = -z \geq 2$.

The left-hand side of (5.6) for $\ell = 2$ reduces to $1024a - 2 \cdot 192 - 65 > 0$. Therefore, this inequality holds. For $\ell \geq 3$ the left-hand side of (5.5) reduces to

$$\begin{aligned} 1024a^{2\ell-3} - 192\ell - 65 &\geq 1024a^\ell - 192\ell - 65 \\ &\geq 1024 \cdot 2^\ell - 192\ell - 65 \\ &\geq 1024\ell - 192\ell - 65 = 832\ell - 65 > 0. \end{aligned}$$

Hence, inequality (5.6) holds.

We turn to the smallest node of the quadrature rule $\widehat{Q}_{2\ell+1}$. It is larger than or equal to -1 if $t_{2\ell+1}(-1) \leq 0$. Using (3.3) this inequality can be expressed as

$$\begin{aligned} &\frac{\frac{1}{2^{\ell+2}} (V_{\ell+2}(-1) + \acute{c} V_{\ell+1}(-1)) - r_{\ell+1} \frac{1}{2^{\ell+1}} (V_{\ell+1}(-1) + \acute{c} V_\ell(-1))}{-1 - \gamma} \overset{\circ}{U}_\ell(-1) \\ &- \widehat{\beta}_{\ell+1} \frac{\frac{1}{2^{\ell+1}} (V_{\ell+1}(-1) + \acute{c} V_\ell(-1)) - r_\ell \frac{1}{2^\ell} (V_\ell(-1) + \acute{c} V_{\ell-1}(-1))}{-1 - \gamma} \overset{\circ}{U}_{\ell-1}(-1) \leq 0. \end{aligned}$$

Substituting the known values of $V_\ell(1)$ and $\overset{\circ}{U}_\ell(1)$ into this inequality gives

$$\begin{aligned} &\frac{\frac{1}{2^{\ell+2}} ((-1)^{\ell+2}(2\ell+5) + \acute{c}(-1)^{\ell+1}(2\ell+3)) - r_{\ell+1} \frac{1}{2^{\ell+1}} ((-1)^{\ell+1}(2\ell+3) + \acute{c}(-1)^\ell(2\ell+1))}{-1 - \gamma} \\ &\quad \times (-1)^\ell \frac{\ell+1}{2^\ell} \\ &- \widehat{\beta}_{\ell+1} \frac{\frac{1}{2^{\ell+1}} ((-1)^{\ell+1}(2\ell+3) + \acute{c}(-1)^\ell(2\ell+1)) - r_\ell \frac{1}{2^\ell} ((-1)^\ell(2\ell+1) + \acute{c}(-1)^{\ell-1}(2\ell-1))}{-1 - \gamma} \\ &\quad \times (-1)^{\ell-1} \frac{\ell}{2^{\ell-1}} \leq 0. \end{aligned}$$

Multiplication by $4^{\ell+1}(-1-\gamma)/((2\ell+3)-(2\ell+1)\acute{c})$ and using that $-1-\gamma < 0$, $\acute{c} \in (-1, 0)$, $(2\ell+3) - (2\ell+1)\acute{c} > 0$, as well as the expression (5.2), yield

$$(L + 2r_{\ell+1})(\ell+1) - \frac{r_{\ell+1}}{r_\ell} \ell(1 + 2Dr_\ell) \leq 0,$$

where

$$L = \frac{2\ell+5 - (2\ell+3)\acute{c}}{2\ell+3 - (2\ell+1)\acute{c}}, \quad D = \frac{2\ell+1 - (2\ell-1)\acute{c}}{2\ell+3 - (2\ell+1)\acute{c}}.$$

Using (5.3), this inequality can be transformed to

$$(\ell + 1) \left(L - \frac{1}{z} \frac{z^{2\ell} + A}{z^{2\ell-2} + A} \right) - \ell \frac{(z^{2\ell} + A)(z^{2\ell-4} + A)}{(z^{2\ell-2} + A)^2} \left(1 - \frac{1}{z} \frac{z^{2\ell-2} + A}{z^{2\ell-4} + A} \cdot D \right) \geq 0.$$

Since $c < 0$ and $\ell \geq 2$, we have

$$z^{2\ell-2} + A \geq 4^{\ell-1} + A > 0, \quad z^{2\ell-2} > 0, \quad A \in \left(-\frac{1}{8}, 0\right), \quad z < 0.$$

After some simplifications and division by $z^{2\ell-1}$, the inequality becomes

$$\begin{aligned} & (\ell(D-1) - 1)(z^{2\ell-2} + Az^{-2} + A) + (\ell(L-1) + L)z^{2\ell-3} - \ell Az - \ell Az^{-3} \\ & + 2LA(\ell+1)z^{-1} + A^2(\ell(L-1) + L)z^{-2\ell+1} + A^2(\ell(D-1) - 1)z^{-2\ell} \leq 0. \end{aligned}$$

This inequality holds due to the following results. The expression for L can be written as

$$L = 1 + \frac{2 - 2\acute{c}}{2\ell + 3 - (2\ell + 1)\acute{c}}.$$

Thus, $1 < L < 2$, as $\acute{c} \in (-1, 0)$ for $c < 0$. Moreover, $0 < D < 1$. Since

$$z^{2\ell-2} + Az^{-2} + A \geq 2^{2\ell-2} - \frac{1}{32} - \frac{1}{8} = 2^{2\ell-2} - \frac{5}{32} > 0,$$

and $\ell(D-1) - 1 < 0$, we have

$$(\ell(D-1) - 1)(z^{2\ell-2} + Az^{-2} + A) < 0.$$

Further,

$$-\ell Az < 0, \quad -\ell Az^{-3} < 0, \quad A^2(\ell(L-1) + L)z^{-2\ell+1} < 0, \quad A^2(\ell(D-1) - 1)z^{-2\ell} < 0.$$

Finally, since $\ell(L-1) + L > 1$, we obtain

$$\begin{aligned} & (\ell(L-1) + L)z^{2\ell-3} + 2LA(\ell+1)z^{-1} < z^{2\ell-3} + 4(\ell+1)\frac{1}{16} \\ & \leq -2^{2\ell-3} + \frac{\ell+1}{4} = -\frac{1}{8}(4^\ell - 2\ell - 2) < 0, \end{aligned}$$

for $\ell \geq 2$. We have shown following result.

THEOREM 5.1. *The NAG quadrature rule $\widehat{Q}_{2\ell+1}$ of the form $(2\ell+2, 2\ell+1, d\sigma_3, d\mu)$, where $d\mu$ is defined by (2.4), is internal, i.e., all its nodes are the in interval $[-1, 1]$, for every $\ell \geq 2$.*

5.1. A numerical example for the measure $d\sigma_3(x)$. We describe an application of the NAG quadrature Gauss rules discussed in Theorem 5.1 to the estimation of the quadrature error in Gauss rules G_ℓ associated with the measure (1.3). The performance of averaged, generalized averaged rules $\widehat{G}_{2\ell+1}$, and truncated generalized averaged rules $Q_{\ell+2}^{(1)}$ has previously been illustrated in [5].

Consider the integral

$$(5.7) \quad I(f) = \int_{-1}^1 f(x) d\sigma_3(x), \quad f(x) = \ln(2-x) \ln(1-x).$$

The integrand is not defined for $x \geq 1$. Since for $c < 0$ in (1.3), the rules $\tilde{G}_{2\ell+1}$ and $\hat{G}_{2\ell+1}$ have a node larger than 1, these rules cannot be used. The truncated rules $Q_{\ell+2}^{(1)}$ are internal and provide error estimates of the correct order of magnitude. Table 5.1 shows the error estimates

$$E_{NAG} = \left| \hat{Q}_{2\ell+1}(f) - G_\ell(f) \right|,$$

$$E_{TGA} = \left| Q_{\ell+2}^{(1)}(f) - G_\ell(f) \right|,$$

for some values of $c < 0$ and ℓ . Observe that the error estimates in the column with header E_{NAG} are closer to the magnitude of the actual quadrature errors than the corresponding estimates in the column with header E_{TGA} . The values of the integral (5.7) are $I(f) \approx -2.2310$ for $c = -0.9$, and $I(f) \approx 1.7717$ for $c = -5$.

TABLE 5.1
 Error estimates E_{TGA} and E_{NAG} , as well as the magnitude of the actual error in the column labeled “Error”.

c	ℓ	E_{TGA}	E_{NAG}	Error
-0.9	5	8.9438(-2)	1.4301(-1)	1.7416(-1)
	10	1.3056(-2)	3.1791(-2)	3.8621(-2)
	15	3.9011(-3)	1.2661(-2)	1.5255(-2)
	20	1.5916(-3)	6.4258(-3)	7.6888(-3)
	25	7.7637(-4)	3.7393(-3)	4.4499(-3)
	30	4.2578(-4)	2.3785(-3)	2.8183(-3)
-5	5	2.9758(-2)	4.3144(-2)	4.8149(-2)
	10	2.7039(-3)	5.8341(-3)	6.5929(-3)
	15	6.2218(-4)	1.7910(-3)	2.0319(-3)
	20	2.1380(-4)	7.7045(-4)	8.7574(-4)
	30	4.6080(-5)	2.3305(-4)	2.6539(-4)
	40	1.5258(-5)	9.9386(-5)	1.1328(-4)

6. Conclusion. The paper [17] introduced two-measure-based generalized Gauss rules that we refer to as NAG rules. They can be applied to estimate the error in Gauss quadrature rules and provide an alternative to averaged and generalized averaged Gauss quadrature rules. Their application is particularly attractive when the NAG rules are internal, but the averaged and generalized averaged Gauss quadrature rules are not, and the integrand only is defined on the convex hull of the support of the measure. This paper investigates the internality of the NAG quadrature rules when used with modified Chebyshev measures. Computed examples show the NAG rules to determine the magnitude of the quadrature error in Gauss rules quite accurately.

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