Journal of Computational and Applied Mathematics 398 (2021) 113696

Contents lists available at ScienceDirect

Journal of Computational and Applied Mathematics

journal homepage: www.elsevier.com/locate/cam

Internality of generalized averaged Gauss quadrature rules and truncated variants for modified Chebyshev measures of the first kind

Dušan Lj. Djukić [a], Rada M. Mutavdžić Djukić [a,*], Lothar Reichel [b], Miodrag M. Spalević [a]

[a] Department of Mathematics, University of Beograd, Faculty of Mechanical Engineering, Kraljice Marije 16, 11120 Belgrade 35, Serbia

[b] Department of Mathematical Sciences, Kent State University, Kent, OH 44242, USA

ARTICLE INFO

Article history:
Received 7 October 2020
Received in revised form 9 May 2021

MSC:
primary 65D30
secondary 65D32

Keywords:
Gauss quadrature
Generalized averaged Gauss quadrature
Truncated generalized averaged Gauss quadrature
Internality of quadrature rule
Modified Chebyshev measure

ABSTRACT

It is desirable that a quadrature rule be internal, i.e., that all nodes of the rule live in the convex hull of the support of the measure. Then the rule can be applied to approximate integrals of functions that have a singularity close to the convex hull of the support of the measure. This paper investigates whether generalized averaged Gauss quadrature formulas for modified Chebyshev measures of the first kind are internal. These rules are applied to estimate the error in Gauss quadrature rules associated with modified Chebyshev measures of the first kind. It is of considerable interest to be able to assess the error in quadrature rules in order to be able to choose a rule that gives an approximation of the desired integral of sufficient accuracy without having to evaluate the integrand at unnecessarily many nodes. Some of the generalized averaged Gauss quadrature formulas considered are found not to be internal. We will show that some truncated variants of these rules are internal, and therefore can be applied to estimate the error in Gauss quadrature rules also when the integrand has singularities on the real axis close to the interval of integration.

1. Introduction

1.1. Gauss quadrature rules

Let $d\lambda$ be a nonnegative measure with infinitely many points of support on the interval $[a, b]$ on the real axis, and assume that all moments are well defined.

By $\{P_k\}_{k=0}^{\infty}$ we denote the set of monic orthogonal polynomials associated with the measure $d\lambda$, where the degree of P_k equals k. Recall that the polynomials P_k satisfy a three-term recurrence relation of the form

$$P_{k+1}(x) = (x - \alpha_k)P_k(x) - \beta_k P_{k-1}(x), \quad k = 1, 2, \ldots, \tag{1}$$

where $P_{-1}(x) \equiv 0$ and $P_0(x) \equiv 1$, and $\beta_k > 0$ for all $k \geq 1$; see, e.g., [1,2] for many properties and examples of orthogonal polynomials.

* Corresponding author.
E-mail addresses: ddjukic@mas.bg.ac.rs (D.Lj. Djukić), rmutavdzic@mas.bg.ac.rs (R.M. Mutavdžić Djukić), reichel@math.kent.edu (L. Reichel), mspalevic@mas.bg.ac.rs (M.M. Spalević).

https://doi.org/10.1016/j.cam.2021.113696
0377-0427/

It is well known that among all interpolatory quadrature rules with n nodes for approximating the integral

$$I(f) = \int_a^b f(x)\,\mathrm{d}\lambda(x), \tag{2}$$

the rule with maximum degree of exactness is the n-node Gauss quadrature rule with respect to the measure $\mathrm{d}\lambda$,

$$Q_n^G(f) = \sum_{i=1}^{n} w_i^{(n)} f(x_i^{(n)}) \tag{3}$$

Its degree of exactness is $2n-1$, that is, $Q_n^G(p) = I(p)$ whenever $p \in \mathcal{P}^{2n-1}$, where $\mathcal{P}^{2n-1}$ denotes the set of polynomials of degree at most $2n-1$.

The nodes $x_i^{(n)}$, $i = 1, 2, \ldots, n$, of the Gauss rule Q_n^G are the zeros of the monic orthogonal polynomial P_n with respect to $\mathrm{d}\lambda$ and lie in the convex hull of the support of $\mathrm{d}\lambda$. The weights $w_i^{(n)}$, $i = 1, 2, \ldots, n$, are known to be positive; see [1,2] for proofs.

In fact, the nodes $x_i^{(n)}$ are the eigenvalues of the $n \times n$ Jacobi matrix

$$J_n = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & \mathbf{0} \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & \\ & \ddots & \ddots & \ddots & \\ & & \sqrt{\beta_{n-2}} & \alpha_{n-2} & \sqrt{\beta_{n-1}} \\ \mathbf{0} & & & \sqrt{\beta_{n-1}} & \alpha_{n-1} \end{bmatrix}, \tag{4}$$

determined by the first $2n-1$ nontrivial recursion coefficients (1), whereas the weights $w_i^{(n)}$ are the square of the first component of suitably normalized eigenvectors; see [1,3] for details. Thus, the matrix (4) together with the moment $\mu_0 = \int_a^b \mathrm{d}\lambda(x)$ determine the Gauss rule Q_n^G. This observation is the basis for the Golub–Welsch algorithm for computing the nodes and weights of an n-node Gauss rule from the $2n-1$ first recursion coefficients (1) in $\mathcal{O}(n^2)$ arithmetic floating point operations (flops); see [4].

1.2. Estimating the error in Gauss rules

It is important to be able to estimate the magnitude of the quadrature error

$$\varepsilon_n(f) = |(I - Q_n^G)(f)|, \tag{5}$$

because this helps to determine a suitable value of n when applying the rule Q_n^G to approximate the integral (2). An unnecessarily large value of n requires the computation of needlessly many nodes and weights, as well as the evaluation of the integrand f at excessively many nodes, while a too small value of n does not yield desired accuracy. The development of methods for estimating the error (5) therefore has received considerable attention over many years.

A popular approach to estimate the error (5) is to use another quadrature rule, A_ℓ, with $\ell > n$ nodes and a degree of exactness higher than $2n-1$. One then can use the difference

$$|(A_\ell - Q_n^G)(f)|$$

as an estimate for (5).

Although letting A_ℓ be the Gauss rule Q_{n+1}^G, whose degree of exactness is $2n+1$, appears to be a natural choice, the error estimate $|(Q_{n+1}^G - Q_n^G)(f)|$ is known to be unreliable; see [5] for a discussion. This has lead to the development of other quadrature formulas for estimating the error (5), among them Gauss–Kronrod rules; see [1] for a discussion of this kind of quadrature rules.

The Gauss–Kronrod quadrature rule associated with the n-node Gauss rule (3) is a nested formula with $2n+1$ nodes - n of the nodes are those of (3), and the remaining nodes are zeros of a Stieltjes polynomial of degree $n+1$. Under suitable conditions, such as when $\mathrm{d}\lambda(x) = \mathrm{d}x$, the zeros of the Stieltjes polynomial are real and are interlaced by the zeros of the Gauss rule (3). Thus, the Gauss–Kronrod rule requires only $n+1$ new function values, in addition to those required to compute $Q_n^G(f)$, and it can be shown to be exact for all polynomials in $\mathcal{P}^{3n+1}$.

However, for many measures, Gauss–Kronrod rules do not have real nodes. This is the case for Gauss–Laguerre and Gauss–Hermite measures (see [6]) and for the Jacobi weight functions $w^{\alpha,\beta}(x) = (1-x)^\alpha(1+x)^\beta$ for $\min(\alpha,\beta) \geqslant 0$ and $\max(\alpha,\beta) > 5/2$ if n is large enough (see [7]). Numerical illustrations can be found in [8]. We refer to [9] for a nice discussion on Gauss–Kronrod rules.

1.3. The averaged rule Q^L_{2n+1} and the generalized averaged rule Q^S_{2n+1}

Another approach to determine a suitable quadrature rule A_ℓ to estimate the error (5) is to construct a new $(n+1)$-node quadrature formula U^θ_{n+1} for approximating the functional

$$I_\theta(f) = I(f) - \theta Q^G_n(f),$$

for some $\theta \in \mathbb{R}$, where $I(f)$ is the integral (2), and use the "stratified" $(2n+1)$-node quadrature formula (i.e. a linear combination of two formulas)

$$Q_{2n+1} = \theta Q^G_n + U^\theta_{n+1} \tag{6}$$

to estimate the error (5); see [10,11] for discussions of this approach. Then the computation of $Q_{2n+1}(f)$ requires the evaluation of the integrand f at only $n+1$ extra nodes, in addition to the evaluation of f at the Gauss nodes $x_i^{(n)}$.

Laurie [12] introduced the $(n+1)$-node anti-Gauss rule Q^A_{n+1} as the Gauss rule approximating I_θ for $\theta = \frac{1}{2}$. Thus $(I - Q^A_{n+1})(p) = -(I - Q^G_n)(p)$ whenever $p \in \mathcal{P}^{2n+1}$. This yields the *averaged rule*, also introduced in [12]:

$$Q^L_{2n+1} = \frac{1}{2}(Q^G_n + Q^A_{n+1}).$$

This rule is exact for all polynomials in $\mathcal{P}^{2n+1}$ and its $n+1$ extra nodes are zeros of

$$F_{n+1} = P_{n+1} - \bar{\beta}_{n+1} P_{n-1}, \tag{7}$$

for $\bar{\beta}_{n+1} = \beta_n$, with β_n a recursion coefficient (1).

For the Laguerre and Hermite weight functions, Ehrich [13] varied θ so as to increase the degree of exactness. By using results in [14] on positive quadrature formulas, Spalević [15,16] proposed a simple numerical method for constructing such a formula for a general nonnegative measure $d\lambda$ for which all required moments exist. This formula, which we will refer to as the *generalized averaged rule* Q^S_{2n+1}, is the optimal formula of type (6), having the degree of exactness (at least) $2n+2$. Its $n+1$ extra nodes are the zeros of the polynomial (7) for $\bar{\beta}_{n+1} = \beta_{n+1}$. Differently from Gauss–Kronrod rules, the quadrature formulas Q^L_{2n+1} and Q^S_{2n+1} are guaranteed to exist, and have real nodes and positive weights. Furthermore, for certain measures $d\lambda$ the rules Q^L_{2n+1} and Q^S_{2n+1} are exact for all polynomials in $\mathcal{P}^{3n+1}$ and, thus, coincide with the Gauss–Kronrod formulas; see [17,18] for examples.

The construction described in [15,16] is as follows. For $0 \leqslant r < n$ we introduce the "reverse" symmetric tridiagonal $(n-r) \times (n-r)$ matrix

$$J^{*(r)}_{n-r} = \begin{bmatrix} \alpha_{n-1} & \sqrt{\beta_{n-1}} & & & \mathbf{0} \\ \sqrt{\beta_{n-1}} & \alpha_{n-2} & \sqrt{\beta_{n-2}} & & \\ & \ddots & \ddots & \ddots & \\ & & \sqrt{\beta_{r+2}} & \alpha_{r+2} & \sqrt{\beta_{r+1}} \\ \mathbf{0} & & & \sqrt{\beta_{r+1}} & \alpha_r \end{bmatrix},$$

and the concatenated symmetric tridiagonal $(2n+1-r) \times (2n+1-r)$ matrix

$$\widehat{J}^{(n-r)}_{2n+1-r} = \begin{bmatrix} J_n & \sqrt{\beta_n} e_n & \mathbf{0} \\ \sqrt{\beta_n} e_n^T & \alpha_n & \sqrt{\bar{\beta}_{n+1}} e_1^T \\ \mathbf{0} & \sqrt{\bar{\beta}_{n+1}} e_1 & J^{*(r)}_{n-r} \end{bmatrix}, \tag{8}$$

where $e_j = [0, \ldots, 0, 1, 0, \ldots, 0]^T$ denotes the jth axis vector of suitable dimension and the superscript ^{T} stands for transposition. Then the matrix (8) together with the moment $\mu_0 = \int_a^b d\lambda$ determine the quadrature rules Q^S_{2n+1} and Q^L_{2n+1} when $\bar{\beta}_{n+1} = \beta_{n+1}$ and $\bar{\beta}_{n+1} = \beta_n$, respectively.

We also refer to [12] for a more efficient method for constructing the rules Q^L_{2n+1}, as well as to [19], where a similarly efficient method for constructing the rules Q^S_{2n+1} recently was proposed.

However, the quadrature rules Q^L_{2n+1} and Q^S_{2n+1} are not guaranteed to be internal, i.e., they may have nodes outside the convex hull H of the support of the measure $d\lambda$. This means that they may yield poor accuracy, or may not be applicable, when the integrand has a singularity close to H. A possible solution to this issue is the *truncated generalized averaged Gauss rules* $Q^{(n-r)}_{2n+1-r}$ determined by the matrix $\widehat{J}^{(n-r)}_{2n+1-r}$ when $\bar{\beta}_{n+1} = \beta_{n+1}$, obtained by "truncating" the Jacobi matrix of Q^S_{2n+1}. Just like the generalized averaged rule Q^S_{2n+1}, they are exact for all polynomials in $\mathcal{P}^{2n+2}$, have real nodes and positive weights. Note that the nodes of $Q^{(n-i)}_{2n+1-i}$ interlace those of $Q^{(n+1-i)}_{2n+2-i}$ for $i = 1, 2, \ldots, r$.

In the present paper, we are concerned with the case $r = n-1$. Then (8) together with the moment μ_0 define the quadrature rule $Q^{(1)}_{n+2}$ with $n+2$ nodes, introduced in [20]. Due to the interlacing property, the truncated rule $Q^{(1)}_{n+2}$ may be internal when Q^S_{2n+1} is not, as illustrated in Section 3.

As noted in [12,15,21], only the two outermost nodes of the rules Q^S_{2n+1}, Q^L_{2n+1}, and $Q^{(1)}_{n+2}$ may be exterior. For certain measures, the internality of these rules is investigated in [17,18,21]. In this paper we discuss the internality of these quadrature rules for modifications of Chebyshev measures of the first kind. Section 2 considers Chebyshev measures of the first kind with a linear divisor and Section 3 is concerned with Chebyshev measures of the first kind with a linear divisor and a linear factor. A few computed examples are presented in Sections 3 and 4 and concluding remarks are provided in Section 5.

2. Modifications by a linear divisor

Henceforth, we let

$$\mathrm{d}\lambda(x) = \frac{\mathrm{d}x}{\sqrt{1-x^2}} \quad \text{for} \quad -1 < x < 1 \tag{9}$$

denote the Chebyshev measure of the first kind. The monic orthogonal polynomials associated with this measure are the polynomials $T_0(x) = 1$ and $\frac{1}{2^{n-1}}T_n(x)$, $n = 1, 2, \ldots$, where the T_n are Chebyshev polynomials of the first kind, characterized by

$$T_n(\cos\xi) = \cos n\xi.$$

Note that $T_n(\pm 1) = (\pm 1)^n$. The recursion coefficients (1) for the polynomials $\frac{1}{2^{n-1}}T_n$ are

$$\alpha_k = 0 \;\; (k \geqslant 0) \quad \text{and} \quad \beta_1 = \frac{1}{2}, \quad \beta_k = \frac{1}{4} \;\; (k \geqslant 2);$$

see, e.g., [1].

This section considers quadrature rules with respect to measures obtained by modifying the measure (9) by a linear divisor. Thus, for a constant $c \in \mathbb{R}\backslash\{0\}$, define the modified Chebyshev measure

$$\mathrm{d}\widetilde{\lambda}(x) = \frac{\mathrm{d}x}{(x-\delta)\sqrt{1-x^2}} \quad \text{for} \quad -1 < x < 1, \tag{10}$$

where $\delta = -\frac{1}{2}(c + c^{-1})$. Due to symmetry, we may assume that $c > 0$ (switching the signs of c and x yields the same measure). We introduce

$$\acute{c} = \min\{c, c^{-1}\}, \quad \text{so that} \quad \delta = -\frac{1}{2}(\acute{c} + \acute{c}^{-1}).$$

Everything in this section will be expressible solely in terms of $\acute{c}$.

The moment

$$\mu_0 = \int_{-1}^{1} \mathrm{d}\widetilde{\lambda}(x) = \frac{2\pi\acute{c}}{1-\acute{c}^2}$$

is not defined for $c = 1$, so we must assume that $c \neq 1$. Then $\delta < -1$.

2.1. Monic orthogonal polynomials

Let $\mathrm{d}\lambda$ and $\mathrm{d}\widetilde{\lambda}$ be measures that satisfy

$$\mathrm{d}\widetilde{\lambda} = \frac{\mathrm{d}\lambda}{x-\delta}.$$

Given the monic orthogonal polynomials P_k and recurrence coefficients α_k, β_k (1) for the measure $\mathrm{d}\lambda$, Gautschi [1, eqs. (2.4.24–25)] gives an algorithm for computing the orthogonal polynomials $\widetilde{P}_k$ and recurrence coefficients $\widetilde{\alpha}_k$, $\widetilde{\beta}_k$ (1) for the measure $\mathrm{d}\widetilde{\lambda}$. The algorithm involves the values

$$r_k = \frac{\rho_{k+1}}{\rho_k}, \quad \text{where} \quad \rho_k = -\int_{-1}^{1} \frac{P_k(x)}{x-\delta}\,\mathrm{d}\lambda(x) \;\; \text{for} \;\; k \geqslant 0, \quad \rho_{-1} = 1,$$

and expresses the polynomials $\widetilde{P}_k$ as

$$\widetilde{P}_k(x) = P_k(x) - r_{k-1}P_{k-1}(x), \quad k \geqslant 1.$$

For the particular measures (9) and (10), we obtain the relations

$$\begin{aligned}
r_k &= \delta - \frac{1}{4r_{k-1}} && (k \geqslant 2),\\
\widetilde{\alpha}_k &= r_k - r_{k-1} && (k \geqslant 1),\\
\widetilde{\beta}_k &= \frac{r_{k-1}}{4r_{k-2}} && (k \geqslant 3),
\end{aligned}$$

with the initial values $r_0 = -\acute{c}$, $r_1 = -\frac{1}{2}\acute{c}$,

$$\widetilde{\alpha}_0 = -\acute{c}, \quad \text{and} \quad \widetilde{\beta}_1 = \frac{1}{2}(1-\acute{c}^2), \quad \widetilde{\beta}_2 = \frac{1}{4}.$$

An easy induction gives us $r_k = -\frac{1}{2}\acute{c}$ for all $k \geqslant 1$.

Theorem 1. *The recurrence coefficients for the monic orthogonal polynomials associated with the measure* $d\widetilde{\lambda}$ (10) *are*

$$\begin{aligned} &\widetilde{\alpha}_0 = -\acute{c}, \quad \widetilde{\alpha}_1 = \tfrac{1}{2}\acute{c}, \qquad &\widetilde{\alpha}_k &= 0 \quad \text{for} \quad k \geqslant 2, \\ &\qquad\qquad \widetilde{\beta}_1 = \tfrac{1}{2}(1-\acute{c}^2), \quad &\widetilde{\beta}_k &= \tfrac{1}{4} \quad \text{for} \quad k \geqslant 2. \end{aligned}$$

The (monic) orthogonal polynomials $\widetilde{P}_k$ *with respect to* $d\widetilde{\lambda}$ *are*

$$\widetilde{P}_k(x) = \frac{1}{2^{k-1}}\left(T_k(x) + \acute{c}\,T_{k-1}(x)\right) \quad \text{for} \quad k \geqslant 2, \tag{11}$$

with $\widetilde{P}_0(x) = 1$ *and* $\widetilde{P}_1(x) = x + \acute{c}$. □

2.2. Internality of generalized averaged Gauss rules and truncated variants

Since the coefficients $\widetilde{\alpha}_k = 0$ and $\widetilde{\beta}_k = \frac{1}{4}$ are constant for $k \geqslant 2$, we obtain as a direct consequence of [22, Theorem 3.1] that:

Theorem 2. *The averaged Gauss formula* Q^L_{2n+1} *and the generalized averaged Gauss formula* Q^S_{2n+1} *associated with the measure* $d\widetilde{\lambda}$ *given by* (10) *both coincide with the Gauss–Kronrod formulas for* $n \geqslant 3$. *Consequently, the polynomials* F_{n+1} *in* (7) *are the Stieltjes polynomials.*

For $n = 1$ the formulas Q^L_{2n+1} and Q^S_{2n+1} do not coincide, whereas for $n = 2$ they coincide, but differ from the Gauss–Kronrod rule.

For $n \geqslant 2$, the quadrature rule $Q_{2n+1} = Q^L_{2n+1} = Q^S_{2n+1}$ has n Gauss nodes (3) and $n+1$ nodes that are the zeros of the polynomial

$$\begin{aligned} F_{n+1}(x) &= \widetilde{P}_{n+1}(x) - \frac{1}{4}\widetilde{P}_{n-1}(x) \\ &= \frac{1}{2^n}\left(T_{n+1}(x) - T_{n-1}(x) + \acute{c}\,(T_n(x) - T_{n-2}(x))\right); \end{aligned}$$

cf. (7). Since $F_{n+1}(\pm 1) = 0$, the outermost zeros of F_{n+1} are at ± 1. This yields the following result.

Theorem 3. *For* $n \geqslant 2$, *the averaged quadrature rule* Q_{2n+1} *associated with the measure* $d\widetilde{\lambda}$ *given by* (10) *is internal. The truncated variants of* Q_{2n+1} *then have all nodes in the open interval* $(-1, 1)$ *and are thus internal as well.*

For $n = 1$, the smallest node of Q^L_3 for all c, as well as the smallest node of Q^S_3 for $\frac{1}{2} < c < 2$, is smaller than -1. On the other hand, the formula Q^S_3 is internal when $c \leqslant \frac{1}{2}$ or $c \geqslant 2$.

3. Modifications by a linear divisor and a linear factor

We consider the measure

$$d\widehat{\lambda}(x) = (x-\gamma)\,d\widetilde{\lambda}(x) = \frac{(x-\gamma)\,dx}{(x-\delta)\sqrt{1-x^2}} \quad \text{for} \quad -1 < x < 1, \tag{12}$$

where $\gamma = -(\frac{1}{2}c + c^{-1})$ and $\delta = -\frac{1}{2}(c + c^{-1})$. Again, switching the signs of c and x if needed, we may assume that $c > 0$.

3.1. Monic orthogonal polynomials

Let $d\widetilde{\lambda}$ and $d\widehat{\lambda}$ be any measures satisfying

$$d\widehat{\lambda}(x) = (x-\gamma)\,d\widetilde{\lambda}(x).$$

Denote by $\widetilde{P}_k, \widetilde{\alpha}_k, \widetilde{\beta}_k$, resp. $\widehat{P}_k, \widehat{\alpha}_k, \widehat{\beta}_k$, the monic orthogonal polynomials and the recurrence coefficients for the measure $d\widetilde{\lambda}$, resp. $d\widehat{\lambda}$.

The polynomials $\widehat{P}_k$ are related to the polynomials $\widetilde{P}_k$ ($k \geqslant 0$) by the following equality from [1, Theorem 1.55]:

$$\widehat{P}_k(x) = \frac{\widetilde{P}_{k+1}(x) - r_k\widetilde{P}_k(x)}{x-\gamma}, \quad \text{where} \quad r_k = \frac{\widetilde{P}_{k+1}(\gamma)}{\widetilde{P}_k(\gamma)}, \tag{13}$$

under the assumption that $\widetilde{P}_k(\gamma) \neq 0$ for all k.

Gautschi [1, eqs. (2.4.12–13)] gives an algorithm for computing the recursion coefficients for the measure $d\widetilde{\lambda}$, given the recursion coefficients for $d\widehat{\lambda}$. With r_k as in (13), we obtain

$$r_0 = \gamma - \widetilde{\alpha}_0, \qquad \widehat{\beta}_0 = -r_0\widetilde{\beta}_0,$$

as well as

$$\begin{aligned} r_k &= \gamma - \widetilde{\alpha}_k - \widetilde{\beta}_k/r_{k-1} && (k > 0),\\ \widehat{\alpha}_k &= \widetilde{\alpha}_{k+1} + r_{k+1} - r_k, &&\\ \widehat{\beta}_k &= \widetilde{\beta}_k r_k/r_{k-1} && (k > 0). \end{aligned}$$

For the particular measures (10) and (12), the initial quantities r_k are given by

$$\begin{aligned} r_0 &= \frac{c^2-2}{2c}, \quad r_1 = -\frac{2}{c(2-c^2)}, \quad r_2 = -\frac{c^4+2c^2+8}{8c} && \text{if } 0 < c < 1,\\ r_0 &= -\frac{c}{2}, \quad r_1 = -\frac{c^4+c^2+2}{2c^3}, \quad r_2 = -\frac{c^6+2c^4+4c^2+4}{2c(c^4+c^2+2)} && \text{if } c > 1, \end{aligned}$$

with

$$r_k = \gamma - \frac{1}{4r_{k-1}} \quad (k \geqslant 2). \tag{14}$$

The initial recursion coefficients are then

$$\begin{cases} \widehat{\alpha}_0 = -\dfrac{c}{2-c^2}, & \widehat{\beta}_1 = \dfrac{2(1-c^2)}{(2-c^2)^2},\\ \widehat{\alpha}_1 = \dfrac{c(c^4+4)}{8(2-c^2)}, & \widehat{\beta}_2 = \dfrac{(2-c^2)(c^4+2c^2+8)}{64}, \end{cases} \quad \text{if } 0 < c < 1,$$

$$\begin{cases} \widehat{\alpha}_0 = -\dfrac{1}{c^3}, & \widehat{\beta}_1 = \dfrac{c^6+c^2-2}{2c^6},\\ \widehat{\alpha}_1 = \dfrac{c^4+4}{2c^3(c^4+c^2+2)}, & \widehat{\beta}_2 = \dfrac{c^2(c^6+2c^4+4c^2+4)}{4(c^4+c^2+2)^2}, \end{cases} \quad \text{if } c > 1,$$

with

$$\widehat{\alpha}_k = r_{k+1} - r_k \quad (k \geqslant 1), \qquad \widehat{\beta}_k = \frac{r_k}{4r_{k-1}} \quad (k \geqslant 2). \tag{15}$$

In order to describe all sequences (r_k) that satisfy the recurrence relation (14), we introduce

$$z = \frac{c^2 + 2 + \sqrt{c^4+4}}{2c}, \tag{16}$$

so that $z^{-1} = \frac{c^2+2-\sqrt{c^4+4}}{2c}$. Note that $z \geqslant \sqrt{2} + 1$, with equality for $c = \sqrt{2}$.

Theorem 4. *Every sequence $(r_k)_{k=1}^{\infty}$ that satisfies (14) with $r_1 \neq -\frac{1}{2}z^{-1}$ is of the form*

$$r_k = -\frac{1}{2} \cdot \frac{z^{k-1} - Az^{1-k}}{z^{k-2} - Az^{2-k}}, \tag{17}$$

where A is a real constant. If $r_1 = -\frac{1}{2}z^{-1}$, then $r_k = -\frac{1}{2}z^{-1}$ for all k. This corresponds to $A = \infty$.

Proof. We will show (17) by induction over k. Letting

$$A = \frac{1 + 2z^{-1}r_1}{1 + 2zr_1} \tag{18}$$

shows that (17) holds for $k = 1$. Let $k \geqslant 2$, assume that (17) holds for $k-1$, and use (14) with $\gamma = -\frac{1}{2}(z + z^{-1})$. We then obtain

$$r_k = -\frac{1}{2}(z + z^{-1}) + \frac{1}{2} \cdot \frac{z^{k-3} - Az^{3-k}}{z^{k-2} - Az^{2-k}} = -\frac{1}{2} \cdot \frac{z^{k-1} - Az^{1-k}}{z^{k-2} - Az^{2-k}}.$$

The initial value $r_1 = -\frac{1}{2}z^{-1}$, obtained by letting $A \to \infty$, clearly gives $r_k = -\frac{1}{2}z^{-1}$ for all k. □

In our case, (18) yields

$$A = \begin{cases} \frac{1}{4}z^{-4}\left(c^2 + \sqrt{c^4+4}\right)^2 & \text{if } c < 1,\\ \frac{1}{4}z^{-2}\left(\sqrt{c^4+4} - c^2\right)^2 & \text{if } c > 1. \end{cases} \tag{19}$$

In either case,

$$0 < A < z^{-2} < 1. \tag{20}$$

From (15) and (17) we obtain the following result.

Theorem 5. *The recursion coefficients for the monic orthogonal polynomials associated with the measure (12) are given by*

$$\widehat{\alpha}_k = -\frac{A(z-z^{-1})^2}{2(z^k - Az^{-k})(z^{k-1} - Az^{1-k})},$$
$$\widehat{\beta}_k = \frac{1}{4} + \frac{A(z-z^{-1})^2}{4(z^{k-1} - Az^{1-k})^2},$$

where z and A are defined by (16) and (19). □

3.2. The averaged Gauss formula Q^L_{2n+1}

The two outermost nodes of the quadrature formula Q^L_{2n+1} are the smallest zero x_1^π and the largest zero x_{n+1}^π of the polynomial

$$\pi_{n+1}(x) = \widehat{P}_{n+1}(x) - \widehat{\beta}_n \widehat{P}_{n-1}(x). \tag{21}$$

The formula Q^L_{2n+1} is internal if and only if $-1 \leqslant x_1^\pi$ and $x_{n+1}^\pi \leqslant 1$. These conditions are equivalent to $x^{n+1}\pi_{n+1}(x) \geqslant 0$ for $x = \pm 1$; see, e.g., [12] for an analogous discussion. It follows that Q^L_{2n+1} is internal if and only if

$$\frac{\widehat{P}_{n+1}(x)}{\widehat{P}_{n-1}(x)} \geqslant \widehat{\beta}_n \quad \text{for} \quad x = \pm 1. \tag{22}$$

Theorem 6. *The quadrature rule Q^L_{2n+1} associated with measure $d\widehat{\lambda}$ (12) has one external node, namely the smallest node.*

Proof. Let $n \geqslant 2$. By (11), (13) and (15), condition (22) reduces to

$$\frac{\frac{1}{2^{n+1}}\left(T_{n+2}(x) + \acute{c}\,T_{n+1}(x)\right) - \frac{r_{n+1}}{2^n}\left(T_{n+1}(x) + \acute{c}\,T_n(x)\right)}{\frac{1}{2^{n-1}}\left(T_n(x) + \acute{c}\,T_{n-1}(x)\right) - \frac{r_{n-1}}{2^{n-2}}\left(T_{n-1}(x) + \acute{c}\,T_{n-2}(x)\right)} \geqslant \frac{r_n}{4r_{n-1}}.$$

For $x = 1$ and $x = -1$, this inequality becomes

$$\frac{1-2r_{n+1}}{1-2r_{n-1}} \geqslant \frac{r_n}{r_{n-1}} \tag{23a}$$

and
$$\frac{1+2r_{n+1}}{1+2r_{n-1}} \geqslant \frac{r_n}{r_{n-1}}, \tag{23b}$$

respectively. Substituting (17) into (23a) and simplifying, we obtain

$$\frac{z^{n-1} - Az^{-n}}{z^{n-3} - Az^{2-n}} \geqslant \frac{(z^{n-1} - Az^{1-n})^2}{(z^{n-2} - Az^{2-n})^2},$$

which reduces to the trivial inequality $A \geqslant -z^{2n-3}$; recall that $z > 0$ and $A > 0$; cf. (20). On the other hand, (23b) reduces to $A \geqslant z^{2n-3}$, which is false by (19) whenever $n \geqslant 2$.

The above statement remains valid for $n = 1$, as can be shown by some straightforward computations. □

Example 1. Table 1 shows the outermost nodes of the averaged Gauss quadrature rule Q^L_{2n+1} for the measure $d\widehat{\lambda}$ (12). The computations for this and the following tables are carried out in Mathematica with high precision arithmetic. The quadrature nodes are computed with the QR algorithm applied to the symmetric tridiagonal matrix associated with the quadrature rule. As expected, the smallest node x_1^π is outside the interval $[-1, 1]$, while the largest node x_{n+1}^π is inside.

3.3. The generalized averaged Gauss formula Q^S_{2n+1}

As in the previous subsection, the two outermost nodes of the quadrature rule Q^S_{2n+1} are the smallest zero x_1^F and the largest zero x_{n+1}^F of the polynomial

$$F_{n+1}(x) = \widehat{P}_{n+1}(x) - \widehat{\beta}_{n+1}\widehat{P}_{n-1}(x). \tag{24}$$

These zeros lie in the interval $[-1, 1]$ if and only if $x^{n+1}F_{n+1}(x) \geqslant 0$ for $x = \pm 1$; see also [15].

Table 1
The smallest zero x_1^π and the largest zero x_{n+1}^π of the polynomial (21).

c	n	x_1^π	x_{n+1}^π
0.1	5	$-1-1.0481(-13)$	$1-8.7604(-14)$
	10	$-1-5.0201(-27)$	$1-4.1536(-27)$
	15	$-1-3.1937(-40)$	$1-2.6335(-40)$
	20	$-1-2.2835(-53)$	$1-1.8797(-53)$
	30	$-1-1.3823(-79)$	$1-1.1360(-79)$
10	5	$-1-5.5711(-13)$	$1-3.7461(-13)$
	10	$-1-2.5196(-23)$	$1-1.6938(-23)$
	15	$-1-1.5192(-33)$	$1-1.0212(-33)$
	20	$-1-1.0305(-43)$	$1-6.9268(-44)$
	30	$-1-5.6191(-64)$	$1-3.7770(-64)$

Table 2
The smallest zero x_1^F and the largest zero x_{n+1}^F of the polynomial (24).

c	n	x_1^F	x_{n+1}^F
0.1	5	$-1-2.0018(-12)$	$1+1.8485(-12)$
	10	$-1-9.5884(-26)$	$1+8.7641(-26)$
	15	$-1-6.1000(-39)$	$1+5.5567(-39)$
	20	$-1-4.3616(-52)$	$1+3.9664(-52)$
	30	$-1-2.6402(-78)$	$1+2.3969(-78)$
10	5	$-1-5.1254(-12)$	$1+4.1956(-12)$
	10	$-1-2.3180(-22)$	$1+1.8971(-22)$
	15	$-1-1.3976(-32)$	$1+1.1438(-32)$
	20	$-1-9.4803(-43)$	$1+7.7580(-43)$
	30	$-1-5.1695(-63)$	$1+4.2302(-63)$

Theorem 7. *The two outermost nodes of the quadrature formula Q^S_{2n+1} for the measure $d\widehat{\lambda}$ given by (12) are both external.*

Proof. In this case, the internality of the nodes x_1^F and x_{n+1}^F is equivalent to

$$\frac{1-2r_{n+1}}{1-2r_{n-1}} \geqslant \frac{r_{n+1}}{r_n} \tag{25a}$$

and
$$\frac{1+2r_{n+1}}{1+2r_{n-1}} \geqslant \frac{r_{n+1}}{r_n}, \tag{25b}$$

respectively. The inequality (25a) for $n \geqslant 2$ reduces to

$$\frac{z^{n-1}-Az^{-n}}{z^{n-3}-Az^{2-n}} \geqslant \frac{z^{n-1}-Az^{1-n}}{z^{n-3}-Az^{3-n}} \cdot \frac{(z^n-Az^{-n})(z^{n-2}-Az^{2-n})}{(z^{n-1}-Az^{1-n})^2},$$

which, when expanded, simplifies to the clearly false inequality $A \leqslant -z^{2n-3}$. Similarly, (25b) reduces to $A \geqslant z^{2n-3}$, which is false as well. □

For $n = 1$, it can be shown that the largest node is internal, whereas the smallest node is external for c approximately between 0.706581 and 1.

Example 2. Table 2 shows the outermost nodes of the generalized averaged Gauss quadrature rule Q^S_{2n+1} for the measure $d\widehat{\lambda}$ (12), computed for several values of n and c. As expected, both outermost nodes x_1^F are x_{n+1}^F lie outside the interval $[-1, 1]$.

3.4. The truncated generalized averaged Gauss formula $Q^{(1)}_{n+2}$

The quadrature rule $Q^{(1)}_{n+2}$ is internal if the smallest zero x_1^t and the largest zero x_{n+2}^t of the polynomial

$$t_{n+2}(x) = (x-\widehat{\alpha}_{n-1})\widehat{P}_{n+1}(x) - \widehat{\beta}_{n+1}\widehat{P}_n(x), \tag{26}$$

belong to the interval $[-1, 1]$; see [21] for a related discussion.

Theorem 8. *For $n \geqslant 3$, the truncated rule $Q^{(1)}_{n+2}$ associated with the measure $d\widehat{\lambda}$ given by (12) is internal.*

Proof. The conditions $x_1^t \geqslant -1$ and $x_{n+2}^t \leqslant 1$ reduce to

$$\frac{-(1+\widehat{\alpha}_{n-1})\widehat{P}_{n+1}(-1)}{\widehat{\beta}_{n+1}\widehat{P}_n(-1)} = 2(1+r_n-r_{n-1}) \cdot \frac{r_n}{r_{n+1}} \cdot \frac{1+2r_{n+1}}{1+2r_n} \geqslant 1 \tag{27a}$$

and

$$\frac{(1-\widehat{\alpha}_{n-1})\widehat{P}_{n+1}(1)}{\widehat{\beta}_{n+1}\widehat{P}_n(1)} = 2(1-r_n+r_{n-1}) \cdot \frac{r_n}{r_{n+1}} \cdot \frac{1-2r_{n+1}}{1-2r_n} \geqslant 1, \tag{27b}$$

respectively. We first verify (27a). Since

$$1 + r_n - r_{n-1} = 1 + \frac{Az^{2n-7}(z^2-1)^2}{2(z^{2n-4}-A)(z^{2n-6}-A)} \geqslant 1,$$

it suffices to show that

$$\frac{r_n}{r_{n+1}} \cdot \frac{1+2r_{n+1}}{1+2r_n} \geqslant \frac{1}{2},$$

i.e., that

$$1 - \frac{r_n}{r_{n+1}} \cdot \frac{1+2r_{n+1}}{1+2r_n} = \frac{Az^{2n-3}(z^2-1)(z+1)}{(z^{2n}-A)(z^{2n-3}+A)} \leqslant \frac{1}{2}.$$

The bounds (20), together with $2A < 1$ and $z > 1$, imply that

$$\begin{aligned}(z^{2n}-A)(z^{2n-3}+A) &\geqslant (z^{2n}-1)z^{2n-3} \\ &= z^{2n-3}(z^2-1)(z^{2n-2}+\cdots+z^2+1) \\ &\geqslant 2Az^{2n-3}(z^2-1)(z+1).\end{aligned}$$

This shows that x_1^t is internal.

Turning to (27b), we have

$$\frac{r_n}{r_{n+1}} \cdot \frac{1-2r_{n+1}}{1-2r_n} = \frac{(z^{2n-2}-A)(z^{2n-1}-A)}{(z^{2n}-A)(z^{2n-3}-A)} = 1 + \frac{Az^{2n-3}(z+1)(z-1)^2}{(z^{2n}-A)(z^{2n-3}-A)} \geqslant 1.$$

It remains to show that $1 - r_n + r_{n-1} \geqslant \frac{1}{2}$, i.e., that

$$r_n - r_{n-1} = \frac{Az^{2n-7}(z^2-1)^2}{2(z^{2n-4}-A)(z^{2n-6}-A)} \leqslant \frac{1}{2}.$$

Using (20) again, we obtain

$$\begin{aligned}(z^{2n-4}-A)(z^{2n-6}-A) &\geqslant z^{-4}(z^{2n-2}-1)(z^{2n-4}-1) \\ &> z^{-4} \cdot z^{2n-4}(z^2-1) \cdot z^{2n-6}(z^2-1) \\ &= z^{2n-5} \cdot z^{-2}z^{2n-7}(z^2-1)^2 \geqslant Az^{2n-7}(z^2-1)^2.\end{aligned}$$

Therefore, x_{n+2}^t is internal as well. □

For $n = 2$, the rule $Q_{n+2}^{(1)}$ is not necessarily internal: its largest node $x_{n+2}^t = x_4^t$ is external for c approximately between 0.94 and 1.06.

Example 3. Table 3 shows the outermost nodes of the truncated generalized averaged Gauss quadrature rule $Q_{n+2}^{(1)}$ for the measure $d\widehat{\lambda}$ (12), computed for several values of n and c. As expected, both outermost nodes x_1^t and x_{n+2}^t lie inside the interval $[-1, 1]$.

4. Numerical performances of the quadrature rules

The following examples illustrate the application of the quadrature rules Q_{2n+1}^L, Q_{2n+1}^S, and $Q_{n+2}^{(1)}$ for estimating the quadrature error (5) in the Gauss quadrature rule Q_n^G. We will compute the integral

$$I(f) = \int_{-1}^{1} f(x)\, d\widehat{\lambda}(x), \tag{28}$$

for two integrands, where the measure $d\widehat{\lambda}$ is given by (12), and tabulate the error estimates

$$\begin{aligned}E_{AG} &= |Q_{2n+1}^L(f) - Q_n^G(f)|, \\ E_{GA} &= |Q_{2n+1}^S(f) - Q_n^G(f)|, \\ E_{TGA} &= |Q_{n+2}^{(1)}(f) - Q_n^G(f)|\end{aligned}$$

Table 3
The smallest zero x_1^t and the largest zero x_{n+2}^t of the polynomial (26).

c	n	x_1^t	x_{n+2}^t
	5	$-9.79038030279709(-1)$	$9.73871633423194(-1)$
	10	$-9.92337134094587(-1)$	$9.91236852047087(-1)$
0.5	15	$-9.96058828954681(-1)$	$9.95661314900172(-1)$
	20	$-9.97604558839063(-1)$	$9.97418577192209(-1)$
	30	$-9.98845880825367(-1)$	$9.98784587481856(-1)$
	5	$-9.77280686318141(-1)$	$9.74518141939028(-1)$
	10	$-9.91951057460943(-1)$	$9.91363145322045(-1)$
2	15	$-9.95917096768783(-1)$	$9.95705465436250(-1)$
	20	$-9.97537626155382(-1)$	$9.97438877010355(-1)$
	30	$-9.98823592963473(-1)$	$9.98791158453879(-1)$

Table 4
The error estimates and the actual *Error* (5).

c	n	E_{AG}	E_{GA}	E_{TGA}	Error	$I(f)$
	5	5.7858	5.7858	5.7394	5.7855	
	10	3.5777(−4)	3.5777(−4)	3.5792(−4)	3.5777(−4)	
0.1	15	7.0202(−11)	7.0202(−11)	7.0205(−11)	7.0202(−11)	1.1220
	20	4.2854(−19)	4.2854(−19)	4.2854(−19)	4.2854(−19)	
	30	1.1955(−38)	1.1955(−38)	1.1955(−38)	1.1955(−38)	
	5	2.9498	2.9498	2.9202	2.9497	
	10	1.8355(−4)	1.8355(−4)	1.8361(−4)	1.8355(−4)	
10	15	3.5798(−11)	3.5798(−11)	3.5799(−11)	3.5798(−11)	5.9317(-1)
	20	2.1753(−19)	2.1753(−19)	2.1753(−19)	2.1753(−19)	
	30	6.0363(−39)	6.0363(−39)	6.0363(−39)	6.0363(−39)	

Table 5
The error estimate E_{TGA} and the actual *Error* (5).

c	n	E_{TGA}	Error	$I(f)$
	5	6.8789(−8)	7.6155(−8)	
	10	4.5475(−10)	6.3826(−10)	
0.5	15	2.2961(−11)	3.9905(−11)	11.9094
	20	2.6705(−12)	5.5638(−12)	
	30	1.2312(−13)	3.4303(−13)	
	5	3.5371(−8)	3.8968(−8)	
	10	2.1419(−10)	2.9828(−10)	
2	15	1.0378(−11)	1.7892(−11)	8.8666
	20	1.1779(−12)	2.4358(−12)	
	30	5.2821(−14)	1.4625(−13)	

for several values of n and $c > 0$. "Error" denotes the actual value of error, estimated using the Gauss quadrature rule with a large number of nodes.

Example 4. Table 4 lists the error estimates when the integrand f in (28) is the entire function

$$f(t) = e^{3t} \sin 10t.$$

All three error estimates are very accurate.

Example 5. Table 5 shows results for the integral (28) with the integrand

$$f(t) = 999.1^{\log_{10}(1+\varepsilon+t)}, \quad \text{where} \quad \varepsilon = 10^{-100}.$$

This integrand has a discontinuity at $t = -1 - \varepsilon$, very close to the support of the measure.

Since the rules Q_{2n+1}^L and Q_{2n+1}^S themselves have a node smaller than $-1-\varepsilon$, they are practically useless in this case. On the other hand, the truncated rule $Q_{n+2}^{(1)}$, which is internal, provides error estimates with the correct order of magnitude.

5. Conclusion

In this paper, we discuss quadrature rules for two kinds of modifications of the Chebyshev measure of the first kind. We study the internality of averaged Gauss rules, generalized averaged Gauss rules, as well as truncated generalized averaged Gauss rules.

Computed examples illustrate the theory, and show the quality of the computed error estimates. The error estimates are found to be very accurate when the integrand does not have a singularity close to the support of the measure. When the integrand has a singularity very close to the support of the measure, the accuracy of the error estimates is reduced.

Acknowledgments

The authors would like to thank the referees for comments that lead to improvements of the presentation. Research of DLD, RMMD, and MMS was supported in part by the Serbian Ministry of Education, Science and Technological Development, according to Contract 451-03-9/2021-14/200105 dated on February 5, 2021. Research by LR was supported in part by National Science Foundation (NSF), USA grant DMS-1729509.

References

[1] W. Gautschi, Orthogonal Polynomials: Computation and Approximation, Oxford University Press, Oxford, 2004.
[2] G. Szegő, Orthogonal Polynomials, fourth ed., Amer. Math. Soc., Providence, RI, 1975.
[3] W. Gautschi, The interplay between classical analysis and (numerical) linear algebra - a tribute to Gene H. Golub, Electron. Trans. Numer. Anal. 13 (2002) 119–147.
[4] G.H. Golub, J.H. Welsch, Calculation of Gauss quadrature rules, Math. Comp. 23 (1969) 221–230.
[5] C.W. Clenshaw, A.R. Curtis, A method for numerical integration on an automatic computer, Numer. Math. 2 (1960) 197–205.
[6] D.K. Kahaner, G. Monegato, Nonexistence of extended Gauss–Laguerre and Gauss–Hermite quadrature rules with positive weights, Z. Angew. Math. Phys. 29 (1978) 983–986.
[7] F. Peherstorfer, K. Petras, Stieltjes polynomials and Gauss–Kronrod quadrature for Jacobi weight functions, Numer. Math. 95 (2003) 689–706.
[8] G.S. Ammar, D. Calvetti, L. Reichel, Computation of Gauss–Kronrod quadrature rules with non-positive weights, Electron. Trans. Numer. Anal. 9 (1999) 26–38.
[9] S. Notaris, Gauss–Kronrod quadrature formulae - a survey of fifty years of research, Electron. Trans. Numer. Anal. 45 (2016) 371–404.
[10] D.P. Laurie, Stratified sequence of nested quadrature formulas, Quaest. Math. 15 (1992) 365–384.
[11] T.N.L. Patterson, Stratified nested and related quadrature rules, J. Comput. Appl. Math. 112 (1999) 243–251.
[12] D.P. Laurie, Anti-Gaussian quadrature formulas, Math. Comp. 65 (1996) 739–747.
[13] S. Ehrich, On stratified extension of Gauss–Laguerre and Gauss–Hermite quadrature formulas, J. Comput. Appl. Math. 140 (2002) 291–299.
[14] F. Peherstorfer, On positive quadrature formulas, Intern. Ser. Numer. Math. 112 (1993) 297–313.
[15] M.M. Spalević, On generalized averaged Gaussian formulas, Math. Comp. 76 (2007) 1483–1492.
[16] M.M. Spalević, A note on generalized averaged Gaussian formulas, Numer. Algorithms 46 (2007) 253–264.
[17] D.Lj. Djukić, L. Reichel, M.M. Spalević, Internality of generalized averaged Gaussian quadrature rules and truncated variants for measures induced by Chebyshev polynomials, Appl. Numer. Math. 142 (2019) 190–205.
[18] D.Lj. Djukić, L. Reichel, M.M. Spalević, J.D. Tomanović, Internality of generalized averaged Gaussian quadrature rules and truncated variants for modified Chebyshev measures of the second kind, J. Comput. Appl. Math. 345 (2019) 70–85.
[19] L. Reichel, M.M. Spalević, A new representation of generalized averaged Gauss quadrature rules, Appl. Numer. Math. 165 (2021) 614–619.
[20] L. Reichel, M.M. Spalević, T. Tang, Generalized averaged Gauss quadrature rules for the approximation of matrix functionals, BIT 56 (2016) 1045–1067.
[21] D.Lj. Djukić, L. Reichel, M.M. Spalević, Truncated generalized averaged Gauss quadrature rules, J. Comput. Appl. Math. 308 (2016) 408–418.
[22] M.M. Spalević, On generalized averaged Gaussian formulas, II, Math. Comp. 86 (2017) 1877–1885.