

Averaged Gauss quadrature formulas: Properties and applications

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Abstract

The estimation of the quadrature error of a Gauss quadrature rule when applied to the approximation of an integral determined by a real-valued integrand and a real-valued nonnegative measure with support on the real axis is an important problem in scientific computing. Laurie developed anti-Gauss quadrature rules as an aid to estimate this error. Under suitable conditions the Gauss and associated anti-Gauss rules give upper and lower bounds for the value of the desired integral. It is then natural to use the average of Gauss and anti-Gauss rules as an improved approximation of the integral. Laurie also introduced these averaged rules. More recently, Spalević derived new averaged Gauss quadrature rules that have higher degree of exactness for the same number of nodes as the averaged rules proposed by Laurie. Numerical experiments reported in this paper show both kinds of averaged rules to often give much higher accuracy than can be expected from their degrees of exactness. This is important when estimating the error in a Gauss rule by an associated averaged rule. We use techniques similar to those employed by Trefethen in his investigation of Clenshaw–Curtis rules to shed light on the performance of the averaged rules. The averaged rules are not guaranteed to be internal, i.e., they may have nodes outside the convex hull of the support of the measure. This paper discusses three approaches to modify averaged rules to make them internal.

Keywords: Gauss quadrature, Gauss–Kronrod quadrature, averaged

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Gauss rules, truncated quadrature rules

AMS classification: Primary 65D30; Secondary 65D32

1. Introduction

Let $d\omega$ be a nonnegative real-valued measure with infinitely many points of support on the real axis, and such that all moments $\mu_k = \int x^k d\omega(x)$, $k = 0, 1, 2, \dots$, exist. We are interested in approximating integrals of the form

$$\mathcal{I}(f) = \int f(x) d\omega(x) \quad (1)$$

by an ℓ -node quadrature rule

$$\mathcal{Q}_\ell(f) = \sum_{k=1}^{\ell} f(x_k^{(\ell)}) w_k^{(\ell)}, \quad (2)$$

with real nodes $x_k^{(\ell)}$ and positive weights $w_k^{(\ell)}$. Gauss quadrature rules are very useful for this purpose. The nodes and weights of the ℓ -node Gauss rule,

$$\mathcal{G}_\ell(f) = \sum_{k=1}^{\ell} f(x_k^{(\ell)}) w_k^{(\ell)}, \quad (3)$$

associated with the measure $d\omega$ are such that the rule is of degree of exactness $2\ell - 1$, i.e.,

$$\mathcal{G}_\ell(f) = \mathcal{I}(f) \quad \forall f \in \mathbb{P}_{2\ell-1}, \quad (4)$$

where $\mathbb{P}_{2\ell-1}$ denotes the set of all polynomials of degree at most $2\ell - 1$. The requirement (4) determines the nodes and weights uniquely. The nodes of the Gauss rule (3) are known to be distinct and to live in the convex hull of the support of $d\omega$, and the weights $w_k^{(\ell)}$ are positive; see, e.g., Gautschi [16] or Szegő [38] for properties of Gauss quadrature formulas.

The Gauss rule (3) can be associated with the symmetric tridiagonal matrix

$$T_\ell = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & 0 \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & \\ & \ddots & \ddots & \ddots & \\ 0 & & \sqrt{\beta_{\ell-2}} & \alpha_{\ell-2} & \sqrt{\beta_{\ell-1}} \\ & & & \sqrt{\beta_{\ell-1}} & \alpha_{\ell-1} \end{bmatrix} \in \mathbb{R}^{\ell \times \ell}, \quad (5)$$

where the $\alpha_k \in \mathbb{R}$ and $\beta_k > 0$ are recursion coefficients for the sequence of monic orthogonal polynomials $\{p_k\}_{k=0}^\infty$ (with $\deg(p_k) = k$) associated with the inner product

$$(g, h) := \int g(x)h(x)d\omega(x)$$

determined by the measure $d\omega$, i.e.,

$$p_{k+1}(x) = (x - \alpha_k)p_k(x) - \beta_k p_{k-1}(x), \quad k = 0, 1, \dots, \quad (6)$$

where $p_{-1}(x) \equiv 0$, $p_0(x) \equiv 1$, and

$$\alpha_k := \frac{(xp_k, p_k)}{(p_k, p_k)}, \quad \beta_k := \frac{(p_k, p_k)}{(p_{k-1}, p_{k-1})}. \quad (7)$$

The coefficients can be conveniently computed for increasing indices by the Stieltjes procedure; see Gautschi [15, 16]. We remark that each coefficient in the sequence $\alpha_0, \beta_1, \alpha_1, \beta_2, \dots, \alpha_{\ell-2}, \beta_{\ell-1}, \alpha_{\ell-1}$ increases the degree of exactness of the quadrature rule (3) associated with the matrix (5) by one. This can be seen by counting the number of moments that are integrated exactly when some coefficients in (5) are perturbed. This observation gives (4).

The eigenvalues of T_ℓ are the nodes and the squared first components of suitably normalized eigenvectors are the weights of \mathcal{G}_ℓ ; see [15, 16, 18]. The Golub–Welsch algorithm [19] is a fairly efficient scheme for computing the nodes and weights of \mathcal{G}_ℓ for a general positive measure $d\omega$. This algorithm requires only $c\ell^2 + \mathcal{O}(\ell)$ arithmetic floating point operations (flops), where $c > 0$ is a fairly small constant that is independent of ℓ ; see also Laurie [28] for a discussion on the computation of nodes and weights for a general positive measure. For special classical measures such as the Legendre, Jacobi, Hermite, and Laguerre measures, and large values of ℓ , faster algorithms are available; see Bogaert [3], Hale and Townsend [20], as well as Glaser et al. [17]. However, in many applications ℓ is not large enough for these algorithms to be competitive.

It is important to be able to estimate the quadrature error

$$\mathcal{I}(f) - \mathcal{G}_\ell(f) \quad (8)$$

to assess whether the number of nodes, ℓ , has been chosen large enough to achieve an approximation of the integral (1) of desired accuracy. Moreover, we would like to avoid to choose ℓ much larger than necessary for the Gauss rule \mathcal{G}_ℓ to achieve the aimed for accuracy. A classical approach to estimate

the error (8) is to evaluate the $(2\ell + 1)$ -node Gauss–Kronrod quadrature rule associated with the ℓ -node Gauss rule (3). The Gauss–Kronrod rule is a quadrature formula of the form

$$\mathcal{K}_{2\ell+1}(f) = \sum_{k=1}^{\ell} f(x_k^{(\ell)}) \widehat{w}_k^{(2\ell+1)} + \sum_{k=\ell+1}^{2\ell+1} f(\widehat{x}_k^{(2\ell+1)}) \widehat{w}_k^{(2\ell+1)}, \quad (9)$$

such that the nodes $x_k^{(\ell)}$, $k = 1, 2, \dots, \ell$, are the nodes of the Gauss rule (3), and the Kronrod nodes $\widehat{x}_k^{(2\ell+1)}$, $k = \ell + 1, \ell + 2, \dots, 2\ell + 1$, and the weights $\widehat{w}_k^{(2\ell+1)}$, $k = 1, 2, \dots, 2\ell + 1$, are determined so that

$$\mathcal{K}_{2\ell+1}(f) = \mathcal{I}(f) \quad \forall f \in \mathbb{P}_{3\ell+1};$$

see Kronrod [24] and Gautschi [14, 15, 16]. Generally, the Kronrod nodes $\widehat{x}_k^{(2\ell+1)}$, $k = \ell + 1, \ell + 2, \dots, 2\ell + 1$, are required to be real and to be interlaced by the Gauss nodes $x_k^{(\ell)}$, $k = 1, 2, \dots, \ell$. In addition, the Gauss–Kronrod weights $\widehat{w}_k^{(2\ell+1)}$, $k = 1, 2, \dots, 2\ell + 1$, should be positive. Efficient numerical methods for computing the nodes and weights of the Gauss–Kronrod rule $\mathcal{K}_{2\ell+1}$ whose nodes $\widehat{x}_k^{(2\ell+1)}$, $k = \ell + 1, \ell + 2, \dots, 2\ell + 1$, and weights $\widehat{w}_k^{(2\ell+1)}$, $k = 1, 2, \dots, 2\ell + 1$, satisfy these conditions are described in [4, 27]. The quadrature error (8) then can be estimated by

$$\mathcal{K}_{2\ell+1}(f) - \mathcal{G}_\ell(f),$$

and the integral (1) can be approximated by $\mathcal{K}_{2\ell+1}(f)$.

However, for many measures $d\omega$, including various Jacobi measures, and for certain numbers of nodes, Gauss–Kronrod rules, whose nodes and weights satisfy the above conditions do not exist; see Notaris [29] for a nice recent survey of Gauss–Kronrod rules and their properties, as well as [23, 32, 33]. The nonexistence of Gauss–Kronrod rules with real nodes and positive weights for important measures prompted the development of other techniques to estimate the error in Gauss quadrature formulas. One such approach is to construct an $(\ell + 1)$ -node quadrature rule $\mathcal{H}_{\ell+1}^{(\theta)}$ for approximating the functional

$$\mathcal{I}^{(\theta)}(f) := \mathcal{I}(f) - \theta \mathcal{G}_\ell(f), \quad (10)$$

and use a linear combination of $\theta \mathcal{G}_\ell(f)$ and $\mathcal{H}_{\ell+1}^{(\theta)}$ for some scalar $\theta \in \mathbb{R}$,

$$\mathcal{Q}_{2\ell+1} = \theta \mathcal{G}_\ell + \mathcal{H}_{\ell+1}^{(\theta)}, \quad (11)$$

to estimate the error $\mathcal{I}(f) - \mathcal{G}_\ell(f)$; see [25, 30] for discussions on this approach. The rule (11) generally has $2\ell + 1$ distinct nodes. The computation of $\mathcal{Q}_{2\ell+1}(f)$ requires the evaluation of the integrand f at only $\ell + 1$ nodes, in addition to the ℓ values of f needed to calculate $\mathcal{G}_\ell(f)$. Thus, the number of required evaluations of the integrand f is the same as for the Gauss–Kronrod rule (9).

A special case of the quadrature formula (11) was proposed by Laurie [26], who introduced the so-called $(\ell + 1)$ -node anti-Gauss rule $\check{\mathcal{G}}_{\ell+1}$ associated with the ℓ -node Gauss rule \mathcal{G}_ℓ . The rule $\check{\mathcal{G}}_{\ell+1}$ is characterized by

$$(\mathcal{I} - \check{\mathcal{G}}_{\ell+1})(f) = -(\mathcal{I} - \mathcal{G}_\ell)(f) \quad \forall f \in \mathbb{P}_{2\ell+1}. \quad (12)$$

This rule corresponds to choosing $\theta = \frac{1}{2}$ in (10) and defining $\mathcal{H}_{\ell+1}^{(\theta)} = \frac{1}{2}\check{\mathcal{G}}_{\ell+1}$ in (11). The quadrature formula (11) then becomes

$$\tilde{\mathcal{A}}_{2\ell+1} := \mathcal{Q}_{2\ell+1} = \frac{1}{2}(\mathcal{G}_\ell + \check{\mathcal{G}}_{\ell+1}), \quad (13)$$

which we refer to as the averaged Gauss rule associated with \mathcal{G}_ℓ . This quadrature rule was first described by Laurie [26].

The property (12) suggests that the quadrature error for $\tilde{\mathcal{A}}_{2\ell+1}$ is smaller than the quadrature error (8) for \mathcal{G}_ℓ . Indeed, it follows from (12) that the degree of exactness of $\tilde{\mathcal{A}}_{2\ell+1}$ is $2\ell + 1$. We will estimate the quadrature error (8) by

$$\tilde{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_\ell(f). \quad (14)$$

The nodes of (13) are the nodes of \mathcal{G}_ℓ as well as the $\ell + 1$ zeros of the polynomial

$$p_{\ell+1}(x) - \eta p_{\ell-1}(x) \quad (15)$$

for $\eta = \beta_\ell$; see Spalević [37] for a proof; the special cases when $d\omega$ is the Hermite or Laguerre measures are discussed by Ehrich [12], and when $d\omega$ is the Gegenbauer measure by Hascelik [22]. Attractions of the averaged Gauss rule (13), when compared to the Gauss–Kronrod rule $\mathcal{K}_{2\ell+1}$, include that the former rule is guaranteed to have real nodes and positive weights, and is easier to compute; see below for comments on computational aspects.

For Gauss–Hermite and Gauss–Laguerre quadrature rules, Ehrich [12] varied θ in (11), or equivalently η in (15), to increase the degree of exactness of the rule (11). He referred to the quadrature rule (11) with θ chosen to give the highest degree of exactness as the optimal averaged Gauss rule.

Using results by Peherstorfer [31] on positive quadrature formulas, Spalević [37] derived a simple method for constructing optimal averaged Gauss rules

associated with the Gauss rule (3) for any nonnegative measure for which all moments exist. Its $\ell + 1$ extra nodes are the zeros of the polynomial (15) with $\eta = \beta_{\ell+1}$. We denote these quadrature rules by $\widehat{\mathcal{A}}_{2\ell+1}$. They have degree of exactness at least $2\ell + 2$. The difference

$$\widehat{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_\ell(f) \tag{16}$$

furnishes an estimate of the quadrature error (8), and the integral (1) can be approximated by $\widehat{\mathcal{A}}_{2\ell+1}(f)$. The optimal averaged quadrature formula $\widehat{\mathcal{A}}_{2\ell+1}$ shares the following advantages of the averaged Gauss rule $\widetilde{\mathcal{A}}_{2\ell+1}$ when compared to the Gauss–Kronrod rule $\mathcal{K}_{2\ell+1}$: the rule $\widehat{\mathcal{A}}_{2\ell+1}$ is guaranteed to have real nodes and positive weights, and is simpler to compute than $\mathcal{K}_{2\ell+1}$.

It is the purpose of the present paper to discuss and illustrate the unexpectedly high accuracy of the averaged and optimal averaged Gauss rules. The high accuracy of the averaged and optimal averaged quadrature rules has, to the best of our knowledge, not been pointed out before. This property is important, because it leads to that (14) and (16) typically furnish quite accurate estimates of (8). The high quality of the estimates (14) and (16) is illustrated by computed examples in subsequent sections, both for integrals that are analytic in a large region in the complex plane that contains the interval of integration, as well as for integrals with integrands that have a singularity close to the interval of integration or at an endpoint of the interval of integration. We find that averaged and optimal averaged quadrature rules typically yield approximations of (1) of higher accuracy than the Gauss quadrature rule of the same degree of exactness.

Hale and Trefethen [21] describe how the accuracy of Gauss rules can be improved by conformal mapping of the convex hull of the support of the measure $d\omega$ onto itself before applying Gauss quadrature. We illustrate how this technique works for averaged and optimal averaged Gauss rules.

It is well known that Gauss quadrature rules are internal, i.e., all nodes live in the convex hull of the support of the measure $d\omega$. However, neither Gauss–Kronrod rules (when they have real nodes) nor averaged and optimal averaged Gauss rules are guaranteed to be internal; they may have real nodes outside the convex hull of the support of the measure. The internality of averaged and optimal averaged Gauss rules has been investigated for a variety of measures; see [7, 8, 9, 10, 11]. In case averaged or optimal averaged Gauss rules are not internal, related internal rules often can be determined by truncating the tridiagonal matrices that are associated with these rules. We describe two truncation techniques, one of which is new, and illustrate their performance.

The averaged Gauss quadrature rule is an average of two quadrature rules. Replacing the average by a weighted average may give an internal quadrature rule, when the averaged rule is not. We describe this approach to determine internal rules and illustrate their use to estimate the error in Gauss rules. Weighted averaged Gauss rules are constructed by numerically effective procedures, in a similar way as the averaged and optimal averaged Gauss rules. Finally, we discuss the application of averaged and optimal averaged Gauss rules when the convex hull of the support of the measure $d\omega$ is a semi-infinite or bi-infinite interval.

This paper is organized as follows. Section 2 reviews the representation of averaged and optimal averaged Gauss rules. Some properties of these rules are described, and computed examples that illustrate the performance and effectiveness of these quadrature formulas are presented. Our analysis is analogous to the discussion on Clenshaw–Curtis rules by Trefethen [39, 41]. Section 3 describes three approaches to modify non-internal averaged and optimal averaged Gauss rules to obtain internal quadrature rules. In Section 4, we discuss the situation when the interval of integration is bi-infinite. Concluding remarks can be found in Section 5.

2. Averaged and optimal averaged Gauss rules

This section first reviews the construction of averaged and optimal averaged Gauss rules. Subsequently, their properties will be discussed and their computational performance will be illustrated.

2.1. The construction of averaged and optimal averaged Gauss rules

Consider the symmetric tridiagonal matrix

$$\check{T}_{\ell+1} = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & & & 0 \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & & & \\ & \ddots & \ddots & \ddots & & & \\ & & \sqrt{\beta_{\ell-2}} & \alpha_{\ell-2} & \sqrt{\beta_{\ell-1}} & & \\ & & & \sqrt{\beta_{\ell-1}} & \alpha_{\ell-1} & \sqrt{2\beta_\ell} & \\ 0 & & & & \sqrt{2\beta_\ell} & \alpha_\ell & \end{bmatrix} \in \mathbb{R}^{(\ell+1) \times (\ell+1)},$$

where the quantities $\alpha_k \in \mathbb{R}$ and $\beta_k > 0$ are recursion coefficients for the sequence of monic orthogonal polynomials (6) associated with the measure $d\omega$. Laurie [26] showed that the eigenvalues of this matrix are the nodes, and the squared first components of suitably normalized eigenvectors are the weights of the anti-Gauss rule $\check{G}_{\ell+1}$ defined by (12).

One of the attractions of the anti-Gauss rule $\check{\mathcal{G}}_{\ell+1}$ and the averaged rule $\tilde{\mathcal{A}}_{2\ell+1}$ is their ease of computation: the symmetric tridiagonal matrix $\tilde{T}_{\ell+1}$ associated with the anti-Gauss rule $\check{\mathcal{G}}_{\ell+1}$ is obtained by multiplying the last off-diagonal elements of the symmetric tridiagonal matrix $T_{\ell+1}$ associated with the Gauss rule $\mathcal{G}_{\ell+1}$ by $\sqrt{2}$; see [26]. The Golub–Welsch algorithm then can be applied to compute the nodes and weights of the anti-Gauss rule $\check{\mathcal{G}}_{\ell+1}$ in $c\ell^2 + \mathcal{O}(\ell)$ flops. Thus, the computational cost of determining the nodes and weights of both the Gauss rule \mathcal{G}_ℓ and the averaged rule $\mathcal{A}_{2\ell+1}$, using the representation (13), is $2c\ell^2 + \mathcal{O}(\ell)$ flops.

Spalević [37] showed that the averaged rule (13) can be represented by a single symmetric tridiagonal matrix of order $2\ell + 1$. This matrix can be determined as follows. Introduce the *reverse matrix*

$$T'_\ell = \begin{bmatrix} \alpha_{\ell-1} & \sqrt{\beta_{\ell-1}} & & & 0 \\ \sqrt{\beta_{\ell-1}} & \alpha_{\ell-2} & \sqrt{\beta_{\ell-2}} & & \\ & \ddots & \ddots & \ddots & \\ 0 & & \sqrt{\beta_2} & \alpha_1 & \sqrt{\beta_1} \\ & & & \sqrt{\beta_1} & \alpha_0 \end{bmatrix} \in \mathbb{R}^{\ell \times \ell},$$

which is obtained by reversing the order of the rows and columns of the matrix (5). The nodes and weights of the averaged Gauss rule (13) are the eigenvalues and the squared first components of suitable normalized eigenvectors, respectively, of the concatenated symmetric tridiagonal matrix

$$\tilde{T}_{2\ell+1} = \begin{bmatrix} T_\ell & \sqrt{\beta_\ell}e_\ell & 0 \\ \sqrt{\beta_\ell}e_\ell^T & \alpha_\ell & \sqrt{\beta_\ell}e_1^T \\ 0 & \sqrt{\beta_\ell}e_1 & T'_\ell \end{bmatrix} \in \mathbb{R}^{(2\ell+1) \times (2\ell+1)}; \quad (17)$$

see [37] for details.

The representation (17) of the averaged Gauss rule (13) is helpful for showing properties of this rule; see, e.g., [7, 8, 9, 10, 11]. However, the computation of the nodes and weights of the averaged rule by applying the Golub–Welsch algorithms to the matrix (17) is more expensive than using the representation (13).

We turn to the construction of optimal averaged Gauss quadrature formulas. Spalević [37] introduced a modification of the matrix (17), in which the elements $\sqrt{\beta_\ell}$ in positions $(\ell + 1, \ell + 2)$ and $(\ell + 2, \ell + 1)$ in (17) are replaced by $\sqrt{\beta_{\ell+1}}$. This yields the matrix

$$\hat{T}_{2\ell+1} = \begin{bmatrix} T_\ell & \sqrt{\beta_\ell}e_\ell & 0 \\ \sqrt{\beta_\ell}e_\ell^T & \alpha_\ell & \sqrt{\beta_{\ell+1}}e_1^T \\ 0 & \sqrt{\beta_{\ell+1}}e_1 & T'_\ell \end{bmatrix} \in \mathbb{R}^{(2\ell+1) \times (2\ell+1)}. \quad (18)$$

The eigenvalues and the squared first component of suitably normalized eigenvectors of this matrix yield the nodes and weights, respectively, of the optimal averaged rule $\widehat{A}_{2\ell+1}$. This choice of the entries $(\ell + 1, \ell + 2)$ and $(\ell + 2, \ell + 1)$ corresponds to the optimal value of η in (15); see [37]. The quadrature formula $\widehat{A}_{2\ell+1}$ therefore is an optimal averaged Gauss rule. Its degree of exactness is at least $2\ell + 2$, which typically is higher than the degree of exactness of the averaged Gauss rule $\widetilde{A}_{2\ell+1}$; see [37] and below. In the special case when the measure $d\omega$ is symmetric with respect to the origin, all recursion coefficients α_j in (6) for the orthogonal polynomials p_j associated with $d\omega$ vanish. Then the degree of exactness of the optimal averaged Gauss rule defined by (18) is at least $2\ell + 3$; see [36, 37] for further details.

The computation of the nodes and weights of $\widehat{A}_{2\ell+1}$ by application of the Golub–Welsch algorithm to the matrix (18) requires $4c\ell^2 + \mathcal{O}(\ell)$ flops. This flop count is higher than for the averaged Gauss rule when using the representation (13). A representation of the quadrature rule $\widehat{A}_{2\ell+1}$ that is analogous to the representation (13) recently has been described in [35]. The computations of the nodes and weights of $\widehat{A}_{2\ell+1}$ using the latter representation is as cheap as computing the nodes and weights of $\widetilde{A}_{2\ell+1}$ using the representation (13).

2.2. Results by Pólya and Bernstein applied to the rules $\widetilde{A}_{2\ell+1}$ and $\widehat{A}_{2\ell+1}$

This subsection is concerned with error bounds for the averaged and optimal averaged quadrature rules. We apply the approach used by Trefethen [39, 41] in his investigation of Clenshaw–Curtis rules to the quadrature formulas $\widetilde{A}_{2\ell+1}$ and $\widehat{A}_{2\ell+1}$.

Consider the interpolatory quadrature formula \mathcal{Q}_ℓ with ℓ nodes (2). Pólya [34] showed that the quadrature error $(\mathcal{I} - \mathcal{Q}_\ell)(f)$ converges to zero as $\ell \rightarrow \infty$ for any function f that is continuous on the convex hull of the support of the measure $d\omega$ if and only if the sums $\sum_{k=1}^{\ell} |w_k^{(\ell)}|$ are uniformly bounded for all ℓ . Since the weights for the quadrature formulas $\widetilde{A}_{2\ell+1}$ and $\widehat{A}_{2\ell+1}$ are positive and sum to $\int d\omega$, convergence of these rules to (1) follows.

A bound for the rate of convergence of the quadrature error can be established by using a result by Bernstein [2]. This result also is discussed by Trefethen [39, Theorem 4.1].

Theorem 1. *Let the convex hull of the support of the measure $d\omega$ be a bounded interval I , which we for notational simplicity assume to be $[-1, 1]$. Let f be continuous on I and let p_ℓ^* denote the best polynomial approximant*

of f on I of degree at most ℓ with respect to the uniform norm. Define

$$E_\ell := \max_{-1 \leq x \leq 1} |f(x) - p_\ell^*(x)|, \quad \ell = 0, 1, 2, \dots \quad (19)$$

Then

$$|(\mathcal{I} - \tilde{\mathcal{A}}_{2\ell+1})(f)| \leq 2\mu_0 E_{2\ell+1}, \quad (20)$$

$$|(\mathcal{I} - \hat{\mathcal{A}}_{2\ell+1})(f)| \leq 2\mu_0 E_{2\ell+2}, \quad (21)$$

where $\mu_0 = \int d\omega$.

Proof. Our proof is analogous to the proof of [39, Theorem 4.1]. We present a proof of (20) for completeness. Since the degree of exactness of the rule

$$\tilde{\mathcal{A}}_{2\ell+1}(f) = \sum_{k=1}^{2\ell+1} f(\tilde{x}_k^{(2\ell+1)}) \tilde{w}_k^{(2\ell+1)}$$

is at least $2\ell + 1$, we have

$$(\mathcal{I} - \tilde{\mathcal{A}}_{2\ell+1})(f) = (\mathcal{I} - \tilde{\mathcal{A}}_{2\ell+1})(f - p_{2\ell+1}^*)$$

and obtain

$$\begin{aligned} |(\mathcal{I} - \tilde{\mathcal{A}}_{2\ell+1})(f)| &= |\mathcal{I}(f - p_{2\ell+1}^*) - \tilde{\mathcal{A}}_{2\ell+1}(f - p_{2\ell+1}^*)| \\ &\leq |\mathcal{I}(f - p_{2\ell+1}^*)| + |\tilde{\mathcal{A}}_{2\ell+1}(f - p_{2\ell+1}^*)| \\ &\leq \mu_0 E_{2\ell+1} + \sum_{k=1}^{2\ell+1} E_{2\ell+1} \tilde{w}_k^{(2\ell+1)}. \end{aligned} \quad (22)$$

Since the weights $\tilde{w}_k^{(2\ell+1)}$ are positive and sum to μ_0 , the error bound (20) follows.

The bound (21) can be shown similarly, by using the fact that the degree of exactness of the rule $\hat{\mathcal{A}}_{2\ell+1}$ is at least $2\ell + 2$. \square

The rate of decay of the error (19) as ℓ increases depends on how many continuous derivatives the function f has on the interval $[-1, 1]$. Bounds are provided, e.g., by [40, Theorems 7.2 and 8.2].

2.3. *Some computed examples with the rules $\tilde{\mathcal{A}}_{2\ell+1}$ and $\hat{\mathcal{A}}_{2\ell+1}$*

Computed examples of this subsection demonstrate that the quadrature errors $(\mathcal{I} - \tilde{\mathcal{A}}_{2\ell+1})(f)$ and $(\mathcal{I} - \hat{\mathcal{A}}_{2\ell+1})(f)$ may be substantially smaller in magnitude than the quadrature error for Gauss rules of the same or higher degree of exactness. This situation is analogous to results reported by Trefethen and Weideman [39, 41, 42] for the Clenshaw–Curtis quadrature rule: The ℓ -node Clenshaw–Curtis quadrature formula has degree of exactness $\ell - 1$, but the quadrature error achieved with this rule often is close to that of the ℓ -node Gauss quadrature formula associated with the measure $d\omega \equiv dx$.

We will use Jacobi weight functions

$$w_{s,t}(x) = (1-x)^s(1+x)^t, \quad -1 < x < 1, \quad s > -1, \quad t > -1, \quad (23)$$

for different values of s and t . All computations reported in this paper are carried out with high-precision arithmetic. Specifically, we have carried out the computations with 110 to 120 significant decimal digits. This is enough to make round-off errors introduced during the computations negligible.

Example 2.1. Consider the integral

$$\mathcal{I}(f) = \int_{-1}^1 f(x) w_{0,0}(x) dx, \quad f(x) = \exp(-x^2), \quad (24)$$

where we note that the integrand is an entire function and $\mathcal{I}(f) \approx 1.4936482$. We supply this value to make it possible to assess the relative quadrature error from Table 1. The integrand is even. Therefore, the degrees of exactness of the rules $\tilde{\mathcal{A}}_{2\ell+1}$ and $\hat{\mathcal{A}}_{2\ell+1}$ are at least $2\ell + 1$ and $2\ell + 3$, respectively. We compare the quadrature error for these rules to the quadrature errors for the $(\ell + 2)$ -node Gauss rule $\mathcal{G}_{\ell+2}$, which has degree of exactness $2\ell + 3$; see (4). Results for the rules \mathcal{G}_ℓ also are displayed.

Table 1 shows the quadrature errors for the quadrature formulas $\tilde{\mathcal{A}}_{2\ell+1}$ and $\hat{\mathcal{A}}_{2\ell+1}$ to be much smaller than for the ℓ -node Gauss rule \mathcal{G}_ℓ , and also smaller than for the $(\ell + 2)$ -node Gauss rule $\mathcal{G}_{\ell+2}$. This high accuracy has not been mentioned and illustrated in the literature before. The table shows the optimal averaged Gauss rules $\hat{\mathcal{A}}_{2\ell+1}$ to give the smallest errors. Since the quadrature error $\mathcal{I}(f) - \hat{\mathcal{A}}_{2\ell+1}(f)$ is much smaller in magnitude than the error $\mathcal{I}(f) - \mathcal{G}_\ell(f)$, the difference $\hat{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_\ell(f)$ provides an accurate approximation of the quadrature error $\mathcal{I}(f) - \mathcal{G}_\ell(f)$. This is illustrated in Tables 1 and 2. These tables also show the error $\mathcal{I}(f) - \mathcal{G}_{\ell+2}(f)$ to be well approximated by $\hat{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_{\ell+2}(f)$.

Table 1: Example 2.1: Results for the integral (24).

ℓ	$\mathcal{I}(f) - \mathcal{G}_\ell(f)$	$\mathcal{I}(f) - \mathcal{G}_{\ell+2}(f)$	$\mathcal{I}(f) - \tilde{\mathcal{A}}_{2\ell+1}(f)$	$\mathcal{I}(f) - \hat{\mathcal{A}}_{2\ell+1}(f)$
5	-1.566(-5)	-2.324(-8)	-1.716(-9)	2.244(-10)
10	5.035(-13)	2.382(-16)	4.567(-18)	-3.059(-19)
15	-1.362(-21)	-3.129(-25)	-2.701(-27)	1.238(-28)
20	7.144(-31)	9.662(-35)	4.723(-37)	-1.653(-38)
30	6.243(-51)	3.933(-55)	8.606(-58)	-2.048(-59)
40	1.935(-72)	7.021(-77)	8.674(-80)	-1.566(-81)

Table 2: Example 2.1: Results for the integral (24).

ℓ	$\tilde{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_\ell(f)$	$\hat{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_{\ell+2}(f)$
5	-1.566(-5)	-2.347(-8)
10	5.035(-13)	2.385(-16)
15	-1.362(-21)	-3.130(-25)
20	7.144(-31)	9.664(-35)
30	6.243(-51)	3.933(-55)
40	1.935(-72)	7.022(-77)

Example 2.2. We approximate the integral

$$\mathcal{I}(f) = \int_{-1}^1 f(x) w_{0,0}(x) dx, \quad f(x) = \exp(-1/x^2), \quad (25)$$

and observe that the integrand is not defined at $x = 0$. However, the limits of the integrand and of all its derivatives as $x \rightarrow 0$ can be defined by continuity to be equal to zero. Quadrature errors are reported in Table 3. They can be seen to be larger than the errors reported in Table 1 for the same values of ℓ . The magnitude of the quadrature errors for the rules $\tilde{\mathcal{A}}_{2\ell+1}$ and $\hat{\mathcal{A}}_{2\ell+1}$ are smaller than the magnitude of the errors for $\mathcal{G}_{\ell+2}$. The quadrature error for the rule $\hat{\mathcal{A}}_{2\ell+1}$ often, but not always, is smaller than the quadrature error for the rule $\tilde{\mathcal{A}}_{2\ell+1}$. The magnitude of the quadrature error for \mathcal{G}_ℓ is larger or smaller than for $\mathcal{G}_{\ell+2}$, depending on ℓ . In particular, the magnitude of the quadrature error does not strictly decrease when ℓ increases.

Similarly as in Example 2.1, the quadrature error $\mathcal{I}(f) - \hat{\mathcal{A}}_{2\ell+1}(f)$ is much smaller in magnitude than the error $\mathcal{I}(f) - \mathcal{G}_\ell(f)$. Therefore, the difference $\hat{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_\ell(f)$ is an accurate approximation of the quadrature error $\mathcal{I}(f) - \mathcal{G}_\ell(f)$. This is illustrated by Tables 3 and 4. These tables also show $\hat{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_{\ell+2}(f)$ to furnish quite accurate estimates of the

Table 3: Example 2.2: Results for the integral (25).

ℓ	$\mathcal{I}(f) - \mathcal{G}_\ell(f)$	$\mathcal{I}(f) - \mathcal{G}_{\ell+2}(f)$	$\mathcal{I}(f) - \tilde{\mathcal{A}}_{2\ell+1}(f)$	$\mathcal{I}(f) - \hat{\mathcal{A}}_{2\ell+1}(f)$
5	7.519(-3)	2.847(-4)	-9.513(-5)	1.040(-4)
10	2.949(-4)	-1.196(-4)	1.467(-6)	1.451(-6)
15	6.002(-6)	-1.613(-5)	-5.101(-9)	-4.470(-9)
20	-1.683(-7)	-2.213(-6)	-3.803(-9)	-3.753(-9)
30	4.238(-8)	-4.534(-8)	1.372(-11)	-1.372(-11)
40	4.935(-9)	8.982(-10)	-7.919(-14)	-9.362(-14)

Table 4: Example 2.2: Results for the integral (25).

ℓ	$\tilde{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_\ell(f)$	$\hat{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_{\ell+2}(f)$
5	7.623(-3)	3.887(-4)
10	2.935(-4)	-1.211(-4)
15	6.006(-6)	-1.612(-5)
20	-1.646(-7)	-2.209(-6)
30	4.237(-8)	-4.535(-8)
40	4.935(-9)	8.983(-10)

quadrature errors $\mathcal{I}(f) - \mathcal{G}_{\ell+2}(f)$ for $\ell \geq 10$.

Example 2.3. We seek to approximate the integral

$$\mathcal{I}(f) = \int_{-1}^1 f(x) w_{0,0}(x) dx, \quad f(x) = \frac{1}{1 + 25x^2}, \quad (26)$$

and have $\mathcal{I}(f) \approx 0.1781477$. The integrand is the Runge function with poles at $\pm i/5$ in the complex plane; here $i := \sqrt{-1}$. Table 5 reports some quadrature errors. We can observe that the quadrature errors for the rules $\tilde{\mathcal{A}}_{2\ell+1}$ and $\hat{\mathcal{A}}_{2\ell+1}$ are much smaller than for the Gauss rules \mathcal{G}_ℓ and $\mathcal{G}_{\ell+2}$ for all ℓ . Note that the quadrature error for $\tilde{\mathcal{A}}_{2\ell+1}$ is smaller than the quadrature error for $\hat{\mathcal{A}}_{2\ell+1}$ for several values of ℓ . We conclude that the rule $\tilde{\mathcal{A}}_{2\ell+1}$ may be competitive with $\hat{\mathcal{A}}_{2\ell+1}$ when the integrand has a pole not far from the convex hull of the support of the measure. Tables 5 and 6 illustrate that the quadrature error $\mathcal{I}(f) - \mathcal{G}_\ell(f)$ can be accurately estimated by $\tilde{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_\ell(f)$ and $\hat{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_\ell(f)$. Similarly, the error $\mathcal{I}(f) - \mathcal{G}_{\ell+2}(f)$ can be accurately estimated by $\tilde{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_{\ell+2}(f)$ and $\hat{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_{\ell+2}(f)$.

Example 2.4. We change the weight function in Example 2.3 and consider

Table 5: Example 2.3: Results for the integral (26).

ℓ	$\mathcal{I}(f) - \mathcal{G}_\ell(f)$	$\mathcal{I}(f) - \mathcal{G}_{\ell+2}(f)$	$\mathcal{I}(f) - \tilde{\mathcal{A}}_{2\ell+1}(f)$	$\mathcal{I}(f) - \hat{\mathcal{A}}_{2\ell+1}(f)$
5	-1.576(-1)	-6.676(-2)	-1.581(-2)	-1.563(-2)
10	1.899(-2)	8.655(-3)	-2.955(-4)	-2.988(-4)
15	-2.653(-3)	-1.197(-3)	-5.595(-6)	-5.451(-6)
20	3.632(-4)	1.641(-4)	-1.041(-7)	-1.125(-7)
30	6.836(-6)	3.088(-6)	-3.152(-11)	-7.999(-11)
40	1.286(-7)	5.808(-8)	3.241(-14)	-3.568(-13)

Table 6: Example 2.3: Results for the integral (26).

ℓ	$\tilde{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_\ell(f)$	$\tilde{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_{\ell+2}(f)$	$\hat{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_\ell(f)$	$\hat{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_{\ell+2}(f)$
5	-1.418(-1)	-5.095(-2)	-1.420(-1)	-5.113(-2)
10	1.928(-2)	8.950(-3)	1.929(-2)	8.954(-3)
15	-2.648(-3)	-1.192(-3)	-2.648(-3)	-1.192(-3)
20	3.633(-4)	1.642(-4)	3.633(-4)	1.642(-4)
30	6.836(-6)	3.088(-6)	6.836(-6)	3.088(-6)
40	1.286(-7)	5.808(-8)	1.286(-7)	5.808(-8)

the approximation of the integral

$$\mathcal{I}(f) = \int_{-1}^1 f(x) w_{-\frac{1}{5}, -\frac{2}{5}}(x) dx, \quad f(x) = \frac{1}{1 + 25x^2}. \quad (27)$$

Then $\mathcal{I}(f) \approx 0.5855375$. Table 7 shows the quadrature error to converge to zero at a similar rate as in Table 5. The quadrature errors for $\tilde{\mathcal{A}}_{2\ell+1}(f)$ and $\hat{\mathcal{A}}_{2\ell+1}(f)$ are smaller than the quadrature errors for $\mathcal{G}_\ell(f)$ and $\mathcal{G}_{\ell+2}(f)$. Table 8 illustrates that both the differences $\tilde{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_\ell(f)$ and $\hat{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_\ell(f)$ give accurate estimates of the error $\mathcal{I}(f) - \mathcal{G}_\ell(f)$, and similarly when $\mathcal{G}_\ell(f)$ is replaced by $\mathcal{G}_{\ell+2}(f)$.

The last few examples of this subsection are from the paper by Clenshaw and Curtis [6], where the authors point out that the difference $\mathcal{G}_{\ell+1}(f) - \mathcal{G}_\ell(f)$ may be a poor estimate of the quadrature error $\mathcal{I}(f) - \mathcal{G}_\ell(f)$. The following examples illustrate that the differences $\tilde{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_\ell(f)$ and $\hat{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_\ell(f)$ provide much more accurate estimates of $\mathcal{I}(f) - \mathcal{G}_\ell(f)$ than $\mathcal{G}_{\ell+1}(f) - \mathcal{G}_\ell(f)$.

Table 7: Example 2.4: Results for the integral (27).

ℓ	$\mathcal{I}(f) - \mathcal{G}_\ell(f)$	$\mathcal{I}(f) - \mathcal{G}_{\ell+2}(f)$	$\mathcal{I}(f) - \tilde{\mathcal{A}}_{2\ell+1}(f)$	$\mathcal{I}(f) - \hat{\mathcal{A}}_{2\ell+1}(f)$
5	-1.678(-1)	-7.140(-2)	-1.624(-2)	-1.610(-2)
10	2.036(-2)	9.278(-3)	-3.068(-4)	-3.092(-4)
15	-2.844(-3)	-1.283(-3)	-5.821(-6)	-5.723(-6)
20	3.893(-4)	1.759(-4)	-1.083(-7)	-1.140(-7)
30	7.327(-6)	3.310(-6)	-3.285(-11)	-6.496(-11)
40	1.378(-7)	6.225(-8)	3.325(-14)	-2.227(-13)

Table 8: Example 2.4: Results for the integral (27).

ℓ	$\tilde{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_\ell(f)$	$\tilde{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_{\ell+2}(f)$	$\hat{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_\ell(f)$	$\hat{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_{\ell+2}(f)$
5	-1.515(-1)	-5.516(-2)	-1.517(-1)	-5.530(-2)
10	2.067(-2)	9.585(-3)	2.067(-2)	9.588(-3)
15	-2.838(-3)	-1.278(-3)	-2.838(-3)	-1.278(-3)
20	3.894(-4)	1.760(-4)	3.894(-4)	1.760(-4)
30	7.327(-6)	3.310(-6)	7.327(-6)	3.310(-6)
40	1.378(-7)	6.225(-8)	1.378(-7)	6.225(-8)

Example 2.5. We consider the integral

$$\mathcal{I}(f) = \int_{-1}^1 f(x) dx, \quad f(x) = \frac{1}{x^4 + x^2 + 0.9}. \quad (28)$$

Its value is $\mathcal{I}(f) \approx 1.5822329$. The approximation of this integral is discussed by Clenshaw and Curtis [6, p. 203]. Table 9 shows the quadrature formulas $\tilde{\mathcal{A}}_{2\ell+1}$ and $\hat{\mathcal{A}}_{2\ell+1}$ to yield much more accurate approximations than \mathcal{G}_ℓ . The former approximations also are more accurate than those delivered by $\mathcal{G}_{\ell+1}$. This is illustrated by Table 10. Table 9 also shows the differences $\mathcal{G}_{\ell+1}(f) - \mathcal{G}_\ell(f)$ and $\tilde{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_\ell(f)$. The latter can be seen to furnish more accurate approximations of the quadrature error $\mathcal{I}(f) - \mathcal{G}_\ell(f)$ than the former. The differences $\tilde{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_\ell(f)$ and $\hat{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_\ell(f)$ agree to 4 significant decimal digits. We therefore do not display the latter differences.

Example 2.6. The integral

$$\mathcal{I}(f) = \int_{-1}^1 f(x) dx, \quad f(x) = \left| x + \frac{1}{2} \right|^{1/2}, \quad (29)$$

is discussed in [6, p. 204]. Its value is approximately 1.46044713. The integrand is not differentiable at the point $x = -\frac{1}{2}$ in the interior of the interval

Table 9: Example 2.5: Results for the integral (28).

ℓ	$\mathcal{I}(f) - \mathcal{G}_\ell(f)$	$\mathcal{I}(f) - \tilde{\mathcal{A}}_{2\ell+1}(f)$	$\mathcal{I}(f) - \hat{\mathcal{A}}_{2\ell+1}(f)$	$\mathcal{G}_{\ell+1}(f) - \mathcal{G}_\ell(f)$	$\tilde{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_\ell(f)$
4	-2.828(-3)	-4.047(-6)	4.912(-7)	-3.781(-3)	-2.823(-3)
8	2.346(-6)	3.377(-10)	-4.962(-10)	3.608(-6)	2.345(-6)
16	-3.835(-12)	-1.692(-18)	-1.128(-16)	-2.360(-12)	-3.835(-12)
32	-7.463(-23)	-1.096(-28)	1.801(-29)	-8.344(-23)	-7.463(-23)
64	6.741(-46)	6.229(-53)	1.616(-52)	5.772(-46)	6.741(-46)

Table 10: Example 2.5: Results for the integral (28).

ℓ	4	8	16	32	64
$\mathcal{I}(f) - \mathcal{G}_{\ell+1}(f)$	9.599(-4)	-1.263(-6)	-1.475(-12)	8.813(-24)	9.690(-47)

of integration, and differently from the situation in Example 2.2, derivatives cannot be defined at $x = -\frac{1}{2}$ by taking limits. The quadrature rules considered in this paper therefore yield poor accuracy when applied to the approximation of (29) in a straightforward manner. This is shown in Table 11, which illustrates that the magnitude of the differences $\tilde{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_\ell(f)$ and $\hat{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_\ell(f)$ are not accurate estimates of the magnitude of the quadrature error $\mathcal{I}(f) - \mathcal{G}_\ell(f)$.

The situation is improved when the integrand is differentiable at all interior points of the interval of integration, but not at an endpoint. To illustrate this, we consider the integral

$$\mathcal{I}(f) = \int_{-1/2}^1 f(x) dx, \quad f(x) = \left(x + \frac{1}{2}\right)^{1/2}, \quad (30)$$

whose value is approximately 1.2247448. Some results for this integral are reported in Tables 12 and 13. The quadrature errors in Table 12 are smaller

Table 11: Example 2.6: Results for the integral (29).

ℓ	$\mathcal{I}(f) - \mathcal{G}_\ell(f)$	$\mathcal{I}(f) - \tilde{\mathcal{A}}_{2\ell+1}(f)$	$\mathcal{G}_{\ell+1}(f) - \mathcal{G}_\ell(f)$	$\tilde{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_\ell(f)$
32	3.170(-3)	2.214(-4)	5.816(-3)	2.948(-3)
128	4.049(-4)	2.806(-5)	7.511(-4)	3.769(-4)

Table 12: Example 2.6: Results for the integral (30).

ℓ	$\mathcal{I}(f) - \mathcal{G}_\ell$	$\mathcal{I}(f) - \tilde{\mathcal{A}}_{2\ell+1}$	$\mathcal{I}(f) - \hat{\mathcal{A}}_{2\ell+1}$
8	-3.103(-4)	-9.356(-6)	-1.011(-5)
32	-5.513(-6)	-1.679(-7)	-1.690(-7)
128	-8.914(-8)	-2.718(-9)	-2.719(-9)

Table 13: Example 2.6: Results for the integral (30).

ℓ	$\mathcal{G}_{\ell+1}(f) - \mathcal{G}_\ell(f)$	$\tilde{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_\ell(f)$	$\hat{\mathcal{A}}_{2\ell+1} - \mathcal{G}_\ell(f)$
8	-8.838(-5)	-3.010(-4)	-3.002(-4)
32	-4.792(-7)	-5.345(-6)	-5.344(-6)
128	-2.049(-9)	-8.643(-8)	-8.643(-8)

than in Table 11. Moreover, Tables 12 and 13 show the estimates $\tilde{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_\ell(f)$ and $\hat{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_\ell(f)$ of the error $\mathcal{I}(f) - \mathcal{G}_\ell(f)$ to be correct to almost two significant decimal digits. In particular, we note that the error estimates $\tilde{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_\ell(f)$ and $\hat{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_\ell(f)$ are much more accurate than the estimate $\mathcal{G}_{\ell+1}(f) - \mathcal{G}_\ell(f)$.

The fact that the quadrature errors reported in Table 12 are smaller than those of Table 11 suggests the splitting

$$\int_{-1}^1 \left| x + \frac{1}{2} \right|^{1/2} dx = \int_{-1}^{-1/2} \left(-x - \frac{1}{2} \right)^{1/2} dx + \int_{-1/2}^1 \left(x + \frac{1}{2} \right)^{1/2} dx,$$

where the integrands of the integrals on the right-hand side are analytic in the interior of the interval of integration. We make the substitution $y = 4x + 3$ in the first integral on the right-hand side, and the substitution $y = \frac{1}{3}(4x - 1)$ in the second integral on the right-hand side. Summing the integrals so obtained gives

$$\mathcal{I}(h) = \int_{-1}^1 h(x) dx, \quad h(x) = \frac{1}{8}(1-x)^{1/2} + \frac{3\sqrt{3}}{8}(1+x)^{1/2}, \quad (31)$$

where we note that the integrand h is not differentiable at the endpoints ∓ 1 of the interval of integration. Tables 14 and 15 report some results. The tables show both the quantities $\tilde{\mathcal{A}}_{2\ell+1}(h) - \mathcal{G}_\ell(h)$ and $\hat{\mathcal{A}}_{2\ell+1}(h) - \mathcal{G}_\ell(h)$ to provide fairly accurate estimates of the quadrature error $\mathcal{I}(h) - \mathcal{G}_\ell(h)$. This example as well as several other computed examples (which we do not

Table 14: Example 2.6: Results for the integral (31).

ℓ	$\mathcal{I}(h) - \mathcal{G}_\ell(h)$	$\mathcal{I}(h) - \tilde{\mathcal{A}}_{2\ell+1}(h)$	$\mathcal{I}(h) - \hat{\mathcal{A}}_{2\ell+1}(h)$
8	-3.700(-4)	-1.116(-5)	-1.206(-5)
32	-6.574(-6)	-2.003(-7)	-2.015(-7)
128	-1.063(-7)	-3.241(-9)	-3.242(-9)

Table 15: Example 2.6: Results for the integral (31).

ℓ	$\mathcal{G}_{\ell+1}(h) - \mathcal{G}_\ell(h)$	$\tilde{\mathcal{A}}_{2\ell+1}(h) - \mathcal{G}_\ell(h)$	$\hat{\mathcal{A}}_{2\ell+1}(h) - \mathcal{G}_\ell(h)$
8	-1.054(-4)	-3.589(-4)	-3.580(-4)
32	-5.715(-7)	-6.373(-6)	-6.372(-6)
128	-2.444(-9)	-1.031(-7)	-1.031(-7)

show) indicate that the error estimates $\tilde{\mathcal{A}}_{2\ell+1}(h) - \mathcal{G}_\ell(h)$ and $\hat{\mathcal{A}}_{2\ell+1}(h) - \mathcal{G}_\ell(h)$ are useful for integrands that are smooth in the interior of the interval of integration, but are nondifferentiable at the interval endpoints.

2.4. Reducing the quadrature error by conformal mapping

The accuracy of the Gauss quadrature formula \mathcal{G}_ℓ can be improved by conformal mapping of the convex hull of the support of the measure $d\omega$ onto itself before application of the quadrature rule; see Hale and Trefethen [21] and Trefethen [41, Sect. 4] for discussions. This technique also can be applied in conjunction with the quadrature formulas $\tilde{\mathcal{A}}_{2\ell+1}$ and $\hat{\mathcal{A}}_{2\ell+1}$ provided that these rules are internal. We illustrate this for the situation when the integrand f is analytic in a small neighborhood of the interval $[-1, 1]$. The new quadrature formula can be derived by transplanting the Gauss quadrature rule \mathcal{G}_ℓ via a conformal map g , with $g([-1, 1]) = [-1, 1]$, of an ellipse with foci ± 1 .

Consider the integral $\int_{-1}^1 f(x) dx$. It can be written as

$$\mathcal{I}(f) = \int_{-1}^1 f(g(s))g'(s) ds. \quad (32)$$

We apply the Gauss rule \mathcal{G}_ℓ in the s -variable. This gives the transformed quadrature formula \mathcal{G}_ℓ^{tr} (see [21, eq. (2.6)]),

$$\mathcal{G}_\ell^{tr}(f) = \sum_{j=1}^{\ell} f(\bar{x}_j^{(\ell)}) \bar{w}_j^{(\ell)}, \quad \bar{x}_j^{(\ell)} = g(x_j^{(\ell)}), \quad \bar{w}_j^{(\ell)} = w_j^{(\ell)} g'(x_j^{(\ell)}),$$

Table 16: Example 2.7: Results for the integral (32).

ℓ	$\mathcal{I}(f) - \mathcal{G}_\ell^{tr}(f)$	$\mathcal{I}(f) - \mathcal{G}_{\ell+2}^{tr}(f)$	$\mathcal{I}(f) - \tilde{\mathcal{A}}_{2\ell+1}^{tr}(f)$	$\mathcal{I}(f) - \hat{\mathcal{A}}_{2\ell+1}^{tr}(f)$
5	-9.476(-3)	1.352(-3)	9.210(-5)	8.523(-5)
10	-8.468(-5)	1.001(-6)	-6.649(-10)	2.589(-8)
15	1.564(-6)	3.082(-7)	3.060(-11)	-1.255(-10)
20	4.121(-8)	-2.681(-8)	-2.670(-13)	2.351(-13)
30	-1.298(-10)	7.792(-11)	-4.874(-16)	-5.044(-16)
40	1.422(-12)	4.537(-14)	9.923(-19)	-3.058(-18)

where $x_j^{(\ell)}$ and $w_j^{(\ell)}$ are the nodes and weights for the untransformed quadrature rule \mathcal{G}_ℓ , respectively. The formulas for the transformed averaged and transformed optimal averaged Gauss rules $\tilde{\mathcal{A}}_{2\ell+1}^{tr}$ and $\hat{\mathcal{A}}_{2\ell+1}^{tr}$, respectively, are analogous.

Example 2.7. Consider the calculation of the integral (32) with $f(x) = \exp(-1/x^2)$. This integral is considered in [41] with the conformal mapping

$$g(s) = 0.5s + 0.2s^3 + 0.3s^5, \quad s \in [-1, 1];$$

see [21, p. 932, Fig. 2.1]. The purpose of the conformal mapping is to increase the number of quadrature nodes near the origin, where the integrand is not analytic. We note that both the averaged Gauss rules $\tilde{\mathcal{A}}_{2\ell+1}$ and the optimal averaged Gauss rules $\hat{\mathcal{A}}_{2\ell+1}$ are internal; see [26, 37].

Table 16 reports quadrature errors for the quadrature formulas \mathcal{G}_ℓ^{tr} , $\mathcal{G}_{\ell+2}^{tr}$, $\tilde{\mathcal{A}}_{2\ell+1}^{tr}$, and $\hat{\mathcal{A}}_{2\ell+1}^{tr}$. The table shows the quadrature rules $\tilde{\mathcal{A}}_{2\ell+1}^{tr}$ to give the highest accuracy in most cases for $\ell \geq 10$. Comparing Table 16 with results reported in Table 3 for the untransformed problem shows the use of conformal mapping to give higher accuracy when ℓ is large.

REMARK 1. In all examples of this section, we have

$$|\mathcal{I}(f) - \mathcal{G}_\ell(f)| > \max\{|\mathcal{I}(f) - \tilde{\mathcal{A}}_{2\ell+1}(f)|, |\mathcal{I}(f) - \hat{\mathcal{A}}_{2\ell+1}(f)|\}.$$

Moreover, for all examples with a sufficiently smooth integrand it holds that

$$|\mathcal{I}(f) - \mathcal{G}_{\ell+2}(f)| > \max\{|\mathcal{I}(f) - \tilde{\mathcal{A}}_{2\ell+1}(f)|, |\mathcal{I}(f) - \hat{\mathcal{A}}_{2\ell+1}(f)|\}.$$

This indicates that it may be advantageous to use the averaged quadrature formulas $\tilde{\mathcal{A}}_{2\ell+1}$ and $\hat{\mathcal{A}}_{2\ell+1}$ instead of the Gauss rules \mathcal{G}_ℓ and $\mathcal{G}_{\ell+2}$ to approximate $\mathcal{I}(f)$.

3. Internality of averaged and optimal averaged Gauss rules

Some nodes of the averaged and optimal averaged Gauss rules $\tilde{\mathcal{A}}_{2\ell+1}$ and $\hat{\mathcal{A}}_{2\ell+1}$ may lie outside the convex hull of the support of the measure $d\omega$. This hampers their applicability when the integrand f only is defined on the convex hull of the support of $d\omega$. We describe three modifications of these rules aimed to yield quadrature rules with all nodes in the convex hull of the support of $d\omega$.

It is well known that the eigenvalues of a real symmetric tridiagonal matrix $S_k \in \mathbb{R}^{k \times k}$ with nonvanishing subdiagonal entries interlace the eigenvalues of the real symmetric tridiagonal matrix $S_{k+1} \in \mathbb{R}^{(k+1) \times (k+1)}$, with leading principal submatrix S_k ; see [43, pp. 103–104]. This suggests that it may be possible to obtain an internal quadrature rule by reducing the order of the matrices (17) and (18). The first approach we consider to is determine interior quadrature rules by removing a few trailing rows and columns from the matrix (18) and, thereby, reduce the number of nodes of the quadrature rule $\hat{\mathcal{A}}_{2\ell+1}$. The order of the matrix $\tilde{\mathcal{A}}_{2\ell+1}$ can be reduced similarly. We refer to quadrature rules determined in this manner as *truncated*.

Introduce the monic polynomials defined by the “shifted” recurrence relation

$$p_{j+1}^{(k)}(x) = (x - \alpha_{j+k})p_j^{(k)}(x) - \beta_{j+k}p_{j-1}^{(k)}(x), \quad j = 0, 1, \dots,$$

with $p_0^{(k)} \equiv 1$ and $p_{-1}^{(k)} \equiv 0$ for the orders $k = 0, 1, \dots$, where the coefficients are given by (7). These polynomials are discussed by Peherstorfer [31, pp. 301–302]. When $k = 0$, we have $p_j^{(0)} \equiv p_j$, $j = 0, 1, \dots$; cf. (6). Polynomials of different orders are related by

$$p_{j+1}^{(k-1)}(x) = (x - \alpha_{k-1})p_j^{(k)}(x) - \beta_k p_{j-1}^{(k+1)}(x), \quad j, k = 1, 2, \dots,$$

and the zeros of the polynomials $p_{j+1}^{(k)}(x)$ and $p_j^{(k+1)}(x)$ for $j, k \geq 0$ are known to interlace; see [31] for details. The polynomials $p_j^{(k)}$ can be used to describe the nodes of the truncated quadrature rules.

Consider the removal of the last r rows and columns of the matrix $\hat{T}_{2\ell+1}$ defined by (18) for some $0 \leq r < \ell$. This gives a symmetric tridiagonal matrix of order $2\ell + 1 - r$ that determines the truncated optimal averaged Gauss rule, which we denote by $\mathcal{Q}_{2\ell+1-r}^{(r)}$. This quadrature formula has the same degree of exactness as $\hat{\mathcal{A}}_{2\ell+1}$ and only $2\ell + 1 - r$ nodes. In particular, $\mathcal{Q}_{2\ell+1}^{(0)} = \hat{\mathcal{A}}_{2\ell+1}$.

Table 17: Example 3.1: Results for the integral (24).

ℓ	$\mathcal{I}(f) - \mathcal{Q}_{\ell+2}^{(\ell-1)}(f)$	$\mathcal{I}(f) - \mathcal{Q}_{\ell+3}^{(\ell-2)}(f)$	$\mathcal{I}(f) - \mathcal{Q}_{2\ell}^{(1)}(f)$	$\mathcal{I}(f) - \mathcal{Q}_{2\ell-2}^{(3)}(f)$
10	2.382(-16)	-4.902(-18)	-3.059(-19)	-3.059(-19)
20	9.662(-35)	-1.067(-36)	-1.653(-38)	-1.653(-38)
30	3.933(-55)	-3.000(-57)	-2.048(-59)	-2.048(-59)
40	7.021(-77)	-4.098(-79)	-1.566(-81)	-1.566(-81)

Table 18: Example 3.2: Results for the integral (27).

ℓ	$\mathcal{I}(f) - \mathcal{Q}_{\ell+3}^{(\ell-2)}(f)$	$\mathcal{I}(f) - \mathcal{Q}_{2\ell}^{(1)}(f)$	$\mathcal{I}(f) - \mathcal{Q}_{2\ell-2}^{(3)}(f)$
10	-6.134(-3)	4.138(-4)	8.705(-4)
20	-1.183(-4)	1.429(-7)	3.053(-7)
30	-2.225(-6)	2.602(-11)	8.352(-11)
40	-4.184(-8)	-1.905(-13)	1.702(-13)

Let $q_{2\ell+1-r}$ denote the nodal polynomial that is associated with the quadrature formula $\mathcal{Q}_{2\ell+1-r}^{(r)}$. It can be written in the form

$$q_{2\ell+1-r} = p_{\ell+1} p_{\ell-r}^{(r)} - \beta_{\ell+1} p_{\ell} p_{\ell-r-1}^{(r)};$$

see [31] for a proof.

Example 3.1. Consider the integral (24). Table 17 reports quadrature errors for several truncated quadrature rules. A comparison with the quadrature errors reported in Table 1 shows the truncated rules $\mathcal{Q}_{\ell+2}^{(\ell-1)}$ and $\mathcal{Q}_{2\ell-2}^{(3)}$ to deliver the same accuracy as the formulas $\mathcal{G}_{\ell+2}$ and $\widehat{\mathcal{A}}_{2\ell+2}$, respectively, to four significant decimal digits. However, while the rule $\widehat{\mathcal{A}}_{2\ell+2}$ has ℓ nodes in common with \mathcal{G}_{ℓ} , the quadrature formulas $\mathcal{Q}_{\ell+2}^{(\ell-1)}$ and $\mathcal{Q}_{2\ell-2}^{(3)}$ do not.

Example 3.2. We determine the quadrature errors for truncated quadrature rules applied to the integral (27). Results are reported in Table 18. A comparison with Table 7 shows the rule $\mathcal{Q}_{\ell+3}^{(\ell-2)}$ to yield slightly smaller quadrature errors than $\mathcal{G}_{\ell+2}$, and the quadrature formulas $\mathcal{Q}_{2\ell}^{(1)}$ and $\mathcal{Q}_{2\ell-2}^{(3)}$ to give about the same accuracy as $\widehat{\mathcal{A}}_{2\ell+1}$.

A different approach to reduce the order of the matrix $\widehat{T}_{2\ell+1}$ in (18) is to remove the first r rows and columns of the submatrix T_{ℓ}' of (18) for some $0 \leq r < \ell$. This determines the truncated quadrature formula $\mathcal{S}_{2\ell+1-r}^{(r)}$, which has the same degree of exactness as $\widehat{\mathcal{A}}_{2\ell+1}$, but only $2\ell + 1 - r$ nodes.

Table 19: Example 3.3: Results for the integral (24).

ℓ	$\mathcal{I}(f) - \mathcal{S}_{2\ell}^{(1)}(f)$	$\mathcal{I}(f) - \mathcal{S}_{2\ell-1}^{(2)}(f)$	$\mathcal{I}(f) - \mathcal{S}_{2\ell-2}^{(3)}(f)$	$\mathcal{I}(f) - \mathcal{S}_{\ell+4}^{(\ell-3)}(f)$
10	-4.932(-19)	-7.665(-19)	-1.188(-18)	-1.344(-17)
20	-2.400(-38)	-3.282(-38)	-4.336(-38)	-5.933(-36)
30	-2.885(-59)	-3.817(-59)	-4.858(-59)	-2.483(-56)
40	-2.174(-81)	-2.832(-81)	-3.546(-81)	-4.494(-78)

In particular, $\mathcal{S}_{2\ell+1}^{(0)} = \widehat{\mathcal{A}}_{2\ell+1}$. Let $s_{2\ell+1-r}$ be the nodal polynomial that is associated with the quadrature formula $\mathcal{S}_{2\ell+1-r}^{(r)}$. This polynomial can be written as

$$s_{2\ell+1-r} = p_{\ell+1}p_{\ell-r} - \beta_{\ell+1}p_{\ell}p_{\ell-r-1};$$

see [31] for a proof.

Example 3.3. Consider the integral (24). Table 19 reports quadrature errors achieved with the rules $\mathcal{S}_{2\ell+1-r}^{(r)}$. A comparison with Table 17 shows the rules $\mathcal{Q}_{2\ell+1-r}^{(r)}$ to give slightly smaller quadrature errors in magnitude for the same values of ℓ and r . The results of this example, as well as numerous other computations, suggest that there is no compelling reason for using the rules $\mathcal{S}_{2\ell+1-r}^{(r)}$ instead of $\mathcal{Q}_{2\ell+1-r}^{(r)}$.

Our last approach to construct internal quadrature rules is to apply modified anti-Gauss rules $\check{\mathcal{G}}_{\ell+1}^{(\gamma)}$. The rule $\check{\mathcal{G}}_{\ell+1}^{(\gamma)}$ has $\ell+1$ nodes and is required to satisfy

$$(\mathcal{I} - \check{\mathcal{G}}_{\ell+1}^{(\gamma)})(f) = -(1 + \gamma)(\mathcal{I} - \mathcal{G})(f) \quad \forall f \in \mathbb{P}_{2\ell+1},$$

for some scalar $\gamma > -1$. This kind of quadrature rules have been discussed in [5, 12, 22]. The special case when $\gamma = 0$ was introduced by Laurie [26]; cf. (12).

Analogously to (13), one can define the weighted averaged Gauss formula

$$\tilde{\mathcal{A}}_{2\ell+1}^{(\gamma)} := \frac{1}{2 + \gamma} \left((1 + \gamma)\mathcal{G}_{\ell} + \check{\mathcal{G}}_{\ell+1}^{(\gamma)} \right). \quad (33)$$

This kind of quadrature formula was first considered by Ehrlich [12] for Laguerre and Hermite measures. Below, we will illustrate how the parameter γ can be used to make the weighted averaged Gauss rule (33) internal for certain measures $d\omega$. We first describe a new representation of the rule (33), and a numerically attractive procedure for its evaluation.

Theorem 2. *The weighted averaged Gauss quadrature rule (33) is associated with the symmetric tridiagonal matrix*

$$\tilde{T}_{2\ell+1}^{(\gamma)} = \begin{bmatrix} T_\ell & \sqrt{\beta_\ell} e_\ell & 0 \\ \sqrt{\beta_\ell} e_\ell^T & \alpha_\ell & \sqrt{\beta} e_1^T \\ 0 & \sqrt{\beta} e_1 & T'_\ell \end{bmatrix} \in \mathbb{R}^{(2\ell+1) \times (2\ell+1)},$$

where

$$\beta = (1 + \gamma)\beta_\ell. \quad (34)$$

Moreover,

$$\tilde{\mathcal{A}}_{2\ell+1}^{(\gamma)} = \frac{\beta}{\beta_\ell + \beta} \mathcal{G}_\ell + \frac{\beta_\ell}{\beta_\ell + \beta} \check{\mathcal{G}}_{\ell+1}^{(\gamma)}, \quad (35)$$

where the quadrature rule $\check{\mathcal{G}}_{\ell+1}^{(\gamma)}$ is associated with the symmetric tridiagonal matrix

$$\check{T}_{\ell+1}^{(\gamma)} = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & & 0 \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & & \\ & \ddots & \ddots & \ddots & & \\ & & \sqrt{\beta_{\ell-2}} & \alpha_{\ell-2} & \sqrt{\beta_{\ell-1}} & \\ 0 & & & \sqrt{\beta_{\ell-1}} & \alpha_{\ell-1} & \sqrt{\beta_\ell + \beta} \\ & & & & \sqrt{\beta_\ell + \beta} & \alpha_\ell \end{bmatrix} \in \mathbb{R}^{(\ell+1) \times (\ell+1)}.$$

Proof. The theorem can be shown by using Proposition 1 and eqs. (3) and (4) in [12]. Alternatively, one can replace $\beta_{\ell+1}$ by β in [35, Theorem 1] and in its proof. \square

The representation (35) can be used to determine the nodes and weights of $\tilde{\mathcal{A}}_{2\ell+1}^{(\gamma)}$ similarly as the computation of the nodes and weights of the averaged Gauss rule by using the representation (13).

To estimate the error $\mathcal{I}(f) - \mathcal{G}_\ell(f)$, we can use the formula

$$\mathcal{I}(f) - \mathcal{G}_\ell(f) \approx \tilde{\mathcal{A}}_{2\ell+1}^{(\gamma)}(f) - \mathcal{G}_\ell(f) = \frac{\beta_\ell}{\beta_\ell + \beta} \left(\check{\mathcal{G}}_{\ell+1}^{(\gamma)}(f) - \mathcal{G}_\ell(f) \right).$$

We conclude this section with discussions on Jacobi and Laguerre weight functions, and show how the parameter γ in (34) in the weighted averaged Gauss rule (13) can be chosen to make the weighted quadrature rules (13) internal.

3.1. The Jacobi weight function

We consider the Jacobi weight function (23), and first derive a condition for the largest zero ζ_{\max} of $\tilde{\mathcal{A}}_{2\ell+1}^{(\gamma)}$ to be in $[-1, 1]$. The inequality $\zeta_{\max} \leq 1$ holds if

$$p_{\ell+1}(1) - \eta p_{\ell-1}(1) \geq 0,$$

which can be written as

$$\eta \leq \frac{p_{\ell+1}(1)}{p_{\ell-1}(1)}. \quad (36)$$

It is known that

$$p_{\ell}(1) = \frac{2^{\ell} \binom{\ell+s}{\ell}}{\binom{2\ell+s+t}{\ell}}, \quad p_{\ell}(-1) = (-1)^{\ell} \frac{2^{\ell} \binom{\ell+t}{\ell}}{\binom{2\ell+s+t}{\ell}}; \quad (37)$$

see [1, 16]. The expression for $p_{\ell}(1)$ and (36) show that $\zeta_{\max} \leq 1$ if

$$\eta \leq 4 \frac{(\ell+s)(\ell+s+1)(\ell+s+t)(\ell+s+t+1)}{(2\ell+s+t-1)(2\ell+s+t)(2\ell+s+t+1)(2\ell+s+t+2)}, \quad (38)$$

and, in particular, that $\zeta_{\max} = 1$ if and only if

$$\eta = 4 \frac{(\ell+s)(\ell+s+1)(\ell+s+t)(\ell+s+t+1)}{(2\ell+s+t-1)(2\ell+s+t)(2\ell+s+t+1)(2\ell+s+t+2)}. \quad (39)$$

The smallest zero ζ_{\min} of $\tilde{\mathcal{A}}_{2\ell+1}^{(\gamma)}$ being in $[-1, 1]$ is equivalent to $p_{\ell+1}(-1) - \eta p_{\ell-1}(-1) \geq 0$ (ℓ is odd), $p_{\ell+1}(-1) - \eta p_{\ell-1}(-1) \leq 0$ (ℓ is even); see [31]. These conditions reduce to

$$\eta \leq \frac{p_{\ell+1}(-1)}{p_{\ell-1}(-1)}. \quad (40)$$

From the equality on the right in (37) and from (40), we conclude that $\zeta_{\min} \geq -1$ if

$$\eta \leq 4 \frac{(\ell+t)(\ell+t+1)(\ell+s+t)(\ell+s+t+1)}{(2\ell+s+t-1)(2\ell+s+t)(2\ell+s+t+1)(2\ell+s+t+2)}. \quad (41)$$

In particular, $\zeta_{\min} = -1$ if and only if

$$\eta = 4 \frac{(\ell+t)(\ell+t+1)(\ell+s+t)(\ell+s+t+1)}{(2\ell+s+t-1)(2\ell+s+t)(2\ell+s+t+1)(2\ell+s+t+2)}.$$

Theorem 3. *The weighted averaged Gauss quadrature formula $\tilde{\mathcal{A}}_{2\ell+1}^{(\gamma)}$ associated with the Jacobi weight function (23) is internal, i.e., $\zeta_{\min} \geq -1$ and $\zeta_{\max} \leq 1$ a) if $s \leq t$ and (38) holds, b) if $s \geq t$ and (41) holds.*

Proof. a) We have that $\zeta_{\max} \leq 1$ if (38) holds. If $s \leq t$, then $(\ell + s)(\ell + s + 1) \leq (\ell + t)(\ell + t + 1)$, i.e., the right-hand side of the inequality (38) is less than or equal to the right-hand side of the inequality (41). Therefore, (41) holds, which implies that $\zeta_{\min} \geq -1$. b) We have that $\zeta_{\min} \geq -1$ if (41) holds. If $s \geq t$, then $(\ell + t)(\ell + t + 1) \leq (\ell + s)(\ell + s + 1)$, i.e., the right-hand side of the inequality (41) is less than or equal to the right-hand side of the inequality (38). Therefore, the inequality (38) holds, which implies that $\zeta_{\max} \leq 1$. \square

Example 3.4. We consider the approximation of the integral

$$\mathcal{I}(f) = \int_{-1}^1 f(x) w_{-\frac{3}{4}, 2}(x) dx, \quad (42)$$

where

$$f(x) = 999.1^{\log_{10}(1-x+\varepsilon)}, \quad w_{-\frac{3}{4}, 2}(x) = \frac{(1+x)^2}{(1-x)^{3/4}},$$

with $\varepsilon = 10^{-6}$. The value of this integral is approximately 1.0495768. The integrand $f(x)$ is defined for $x < 1 + 10^{-6}$. Graphs in [26] and [37] indicate that both the largest and smallest nodes of the quadrature rules $\mathcal{A}_{2\ell+1}$ and $\hat{\mathcal{A}}_{2\ell+1}$ are outside of the interval $[-1, 1]$. Numerical tests confirmed this. For the values of ℓ reported in Table 20, we found that the largest nodes of $\tilde{\mathcal{A}}_{2\ell+1}$ and $\hat{\mathcal{A}}_{2\ell+1}$ to be larger than $1 + \varepsilon$, which means that the integral $\mathcal{I}(f)$ cannot be approximated by these quadrature rules. For this reason, we use the weighted averaged Gauss quadrature formula $\tilde{\mathcal{A}}_{2\ell+1}^{(\gamma)}$ with η given by (39) (for $s = -0.75$ and $t = 2$). The so obtained quadrature rule is of Radau type, i.e., its largest node is $+1$. Some results are reported in Table 20; which shows the differences $\tilde{\mathcal{A}}_{2\ell+1}^{(\gamma)}(f) - \mathcal{G}_\ell(f)$ to be quite accurate approximations of $\mathcal{I}(f) - \mathcal{G}_\ell(f)$.

3.2. Laguerre weight functions

We consider Laguerre weight functions

$$w^{(\alpha)}(x) = x^\alpha e^{-x}, \quad 0 \leq x < \infty, \quad \alpha > -1.$$

The monic orthogonal polynomials associated with these weight functions satisfy

$$p_\ell(0) = (-1)^\ell \ell! \binom{\ell + \alpha}{\ell};$$

Table 20: Example 3.4: Results for the integral (42).

ℓ	$\mathcal{I}(f) - \mathcal{G}_\ell(f)$	$\tilde{\mathcal{A}}_{2\ell+1}^{(\gamma)}(f) - \mathcal{G}_\ell(f)$
5	-8.264(-8)	-7.876(-8)
10	-1.302(-9)	-1.220(-9)
15	-1.101(-10)	-1.025(-10)
20	-1.862(-11)	-1.727(-11)

see [1]. In a similar way as for the Jacobi measure, we conclude that the smallest zero of ζ_{\min} of $\tilde{\mathcal{A}}_{2\ell+1}^{(\gamma)}$ is nonnegative if

$$\eta \leq (\ell + \alpha)(\ell + \alpha + 1) \quad (43)$$

and, in particular, that $\zeta_{\min} = 0$ if and only if

$$\eta = (\ell + \alpha)(\ell + \alpha + 1). \quad (44)$$

Theorem 4. *The averaged Gauss quadrature formula $\tilde{\mathcal{A}}_{2\ell+1}$ defined by (13) is internal.*

Proof. We have that $\beta_\ell = \ell(\ell + \alpha)$; see [1]. Therefore, letting $\eta = \beta_\ell$ in (43), we obtain that $\ell \leq \ell + \alpha + 1$ ($\alpha > -1$). This shows that $\tilde{\mathcal{A}}_{2\ell+1}$ is internal; see also [26, Th. 2(2)]. \square

For the optimal averaged Gauss quadrature formula $\hat{\mathcal{A}}_{2\ell+1}$, we have that $\beta_{\ell+1} = (\ell+1)(\ell+1+\alpha)$; see [1]. Letting $\eta = \beta_{\ell+1}$ in (43), we get $\alpha \geq 1$. This is the condition for internality of $\hat{\mathcal{A}}_{2\ell+1}$. This means that for $-1 < \alpha < 1$, the smallest node of $\hat{\mathcal{A}}_{2\ell+1}$ is negative.

Example 3.5. Consider the integral

$$\mathcal{I}(f) = \int_0^\infty f(x)w^{(-1/2)}(x)dx, \quad f(x) = \exp(\arctan(x + 70)), \quad (45)$$

whose value is about 8.4062581. By Theorem 4 the rule $\tilde{\mathcal{A}}_{2\ell+1}$ is internal, but the formula $\hat{\mathcal{A}}_{2\ell+1}$ is not; its smallest node is negative. The quadrature rule $\tilde{\mathcal{A}}_{2\ell+1}^{(\gamma)}$ with η given by (44) and $\alpha = -1/2$ is of Radau type, i.e., its smallest node is zero. A few computed results are reported in Table 21.

Example 3.6. We consider the calculation of the integral

$$\mathcal{I}(f) = \int_0^\infty f(x)w^{(-1/2)}(x)dx, \quad f(x) = 99999.1^{\log_{10}(x+\varepsilon)}, \quad \varepsilon = 10^{-3}, \quad (46)$$

Table 21: Example 3.5: Results for the integral (45).

ℓ	$\mathcal{I}(f) - \mathcal{G}_\ell(f)$	$\mathcal{I}(f) - \check{\mathcal{G}}_{\ell+1}^{(\gamma)}(f)$	$\mathcal{I}(f) - \tilde{\mathcal{A}}_{2\ell+1}(f)$	$\mathcal{I}(f) - \hat{\mathcal{A}}_{2\ell+1}(f)$	$\mathcal{I}(f) - \tilde{\mathcal{A}}_{2\ell+1}^{(\gamma)}(f)$
5	-6.752(-17)	7.412(-17)	-9.615(-20)	1.551(-20)	-7.225(-20)
10	-2.162(-27)	2.263(-27)	-4.462(-30)	1.185(-30)	-3.156(-30)
15	-4.107(-17)	4.230(-36)	-9.836(-39)	3.500(-39)	-6.673(-39)
20	-9.086(-44)	9.282(-44)	-2.335(-46)	1.015(-46)	-1.531(-46)
30	-4.825(-57)	4.889(-57)	-1.302(-59)	7.397(-60)	-8.056(-60)
40	-1.562(-68)	1.576(-68)	-4.213(-71)	2.855(-71)	-2.484(-71)

Table 22: Example 3.6: Results for the integral (46).

ℓ	$\mathcal{I}(f) - \mathcal{G}_\ell(f)$	$\mathcal{I}(f) - \check{\mathcal{G}}_{\ell+1}(f)$	$\mathcal{I}(f) - \tilde{\mathcal{A}}_{2\ell+1}(f)$	$\mathcal{I}(f) - \tilde{\mathcal{A}}_{2\ell+1}^{(\gamma)}(f)$
5	-3.462(-8)	3.636(-8)	-1.841(-9)	-8.160(-10)
10	-2.859(-10)	2.893(-10)	-2.152(-11)	-5.311(-12)
15	-2.331(-11)	2.344(-11)	-1.883(-12)	-3.188(-13)
20	-4.193(-12)	4.207(-12)	-3.487(-13)	-4.474(-14)

whose value is about 52.4006396. The integrand is defined for $x > -\varepsilon$, and the rule $\tilde{\mathcal{A}}_{2\ell+1}$ is internal by Theorem 4, while the rule $\hat{\mathcal{A}}_{2\ell+1}$ is not. Straightforward computations show that for the values of ℓ reported in Table 22, the smallest node of $\hat{\mathcal{A}}_{2\ell+1}$ is smaller than $-\varepsilon$. Hence, the integral (46) cannot be approximated by these quadrature formulas. The rule $\tilde{\mathcal{A}}_{2\ell+1}^{(\gamma)}$ with η given by (44) with $\alpha = -1/2$ is of Radau type, i.e., its first node is zero. A few computed results are reported in Table 22. The rule $\tilde{\mathcal{A}}_{2\ell+1}^{(\gamma)}$ can be seen to be more accurate than the rule $\tilde{\mathcal{A}}_{2\ell+1}$ for all values of ℓ .

4. Averaged and optimal averaged Gauss rules for a bi-infinite interval

This section discusses several ways to approximate integrals determined by a measure with support on the entire real axis.

Example 4.1. We consider the approximation of the integral

$$\mathcal{I}(f) = \int_{-\infty}^{+\infty} f(x) w_{2/3}(x) dt, \quad f(x) = \exp(-x^2), \quad (47)$$

with the Hermite weight function $w_\mu(x) = |x|^\mu \exp(-x^2)$ for $\mu = 2/3$. The value of the integral is about 0.4132519. Some results are reported in Ta-

Table 23: Example 4.1: Results for the integral (47).

ℓ	$\mathcal{I}(f) - \mathcal{G}_\ell(f)$	$\mathcal{I}(f) - \mathcal{G}_{\ell+2}(f)$	$\mathcal{I}(f) - \tilde{\mathcal{A}}_{2\ell+1}(f)$	$\mathcal{I}(f) - \hat{\mathcal{A}}_{2\ell+1}(f)$
5	-9.727(-3)	-1.260(-3)	-6.359(-4)	-4.970(-4)
10	4.953(-5)	6.186(-6)	-2.853(-6)	-2.149(-8)
20	1.313(-9)	1.553(-10)	-3.841(-11)	-4.672(-13)
30	2.901(-14)	3.363(-15)	-5.685(-16)	-7.882(-18)
40	5.938(-19)	6.814(-20)	-8.749(-21)	-1.290(-22)

Table 24: Example 4.2: Results for the integral (48).

ℓ	$\mathcal{I}(f) - \mathcal{G}_\ell(f)$	$\mathcal{I}(f) - \mathcal{G}_{\ell+2}(f)$	$\mathcal{I}(f) - \tilde{\mathcal{A}}_{2\ell+1}(f)$	$\mathcal{I}(f) - \hat{\mathcal{A}}_{2\ell+1}(f)$
12	9.423(-5)	-2.292(-5)	-1.975(-6)	-1.530(-6)
24	1.524(-9)	-1.385(-9)	-3.283(-11)	-9.567(-11)
50	1.922(-18)	7.299(-19)	4.058(-22)	4.011(-20)
100	-1.636(-35)	4.118(-36)	3.934(-38)	3.216(-38)

Table 23. The table shows the rule $\hat{\mathcal{A}}_{2\ell+1}$ to yield the highest accuracy. In particular, this rule is more accurate than $\mathcal{G}_{\ell+2}$.

Example 4.2. We approximate the integral

$$\mathcal{I}(f) = \int_{-\infty}^{+\infty} f(x) w_0(x) dx, \quad f(x) = \cos(x^2), \quad w_0(x) = \exp(-x^2), \quad (48)$$

with exact value

$$\frac{1}{2} \left((1 + \sqrt{2})\pi \right)^{1/2} \approx 1.3769963.$$

Some results are displayed in Table 24. Table 25 shows the differences $\tilde{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_\ell(f)$ and $\hat{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_\ell(f)$. These differences are seen to be quite accurate estimates of the actual quadrature error in $\mathcal{G}_\ell(f)$.

Example 4.3. We calculate the integral

$$\mathcal{I}(f) = \int_{-\infty}^{+\infty} f(x) w_0(x) dx, \quad f(x) = \cos(x^3), \quad w_0(x) = \exp(-x^2). \quad (49)$$

The exact value is

$$\frac{2e^{2/27} K_{1/3} \left(\frac{2}{27} \right)}{3\sqrt{3}} \approx 1.3881082,$$

where K_ν is the modified Bessel function of the second kind of order ν . Some results are reported in Table 26. The table shows Gauss–Hermite

Table 25: Example 4.2: Results for the integral (48).

ℓ	$\tilde{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_\ell(f)$	$\hat{\mathcal{A}}_{2\ell+1}(f) - \mathcal{G}_\ell(f)$
12	9.621(-5)	9.576(-5)
24	1.557(-9)	1.619(-9)
50	-2.786(-18)	-2.825(-18)
100	-1.640(-35)	-1.639(-35)

Table 26: Example 4.3: Results for the integral (49).

ℓ	$\mathcal{I}(f) - \mathcal{G}_\ell(f)$	$\mathcal{I}(f) - \mathcal{G}_{\ell+2}(f)$	$\mathcal{I}(f) - \tilde{\mathcal{A}}_{2\ell+1}(f)$	$\mathcal{I}(f) - \hat{\mathcal{A}}_{2\ell+1}(f)$
25	-1.554(-2)	-4.977(-3)	1.120(-4)	-1.777(-4)
50	9.443(-4)	-9.295(-4)	-4.219(-6)	1.651(-7)
75	-3.714(-4)	-2.679(-5)	2.164(-7)	-1.796(-6)
100	7.769(-5)	1.110(-4)	4.504(-8)	5.236(-7)

quadrature not to perform well: We can see the quadrature errors for the Gauss rule $\mathcal{G}_{\ell+2}$ to be larger for some values of ℓ than the quadrature errors for \mathcal{G}_ℓ , though the quadrature errors for the averaged and optimal averaged Gauss rules $\tilde{\mathcal{A}}_{2\ell+1}$ and $\hat{\mathcal{A}}_{2\ell+1}$ are smaller than for both \mathcal{G}_ℓ and $\mathcal{G}_{\ell+2}$ for all values of ℓ .

The inefficiency of Gauss–Hermite quadrature for large ℓ is discussed and illustrated by Trefethen [41, p. 9]. Trefethen [41, §5] suggests an approach to compute more accurate approximations of the integral (49) based on ignoring contributions to the integral for $|x| > \delta$. Thus,

$$\begin{aligned} \mathcal{I}(f) &= \int_{-\infty}^{+\infty} \cos(x^3) e^{-x^2} dx \approx \int_{-\delta}^{\delta} \cos(x^3) e^{-x^2} dx \\ &= \int_{-1}^1 \left[\delta \cos(\delta^3 x^3) e^{-\delta^2 x^2} \right] dx \end{aligned} \quad (50)$$

with $\delta = O(\ell^{1/3})$, where the last integral is approximated by Gauss–Legendre quadrature rules \mathcal{G}_ℓ^t applied to the integrand $\delta \cos(\delta^3 x^3) e^{-\delta^2 x^2}$. In the computations reported in Table 27, we use $\delta = \ell^{1/3}$. We similarly define the averaged and optimal averaged Gauss rules $\tilde{\mathcal{A}}_{2\ell+1}^t$ and $\hat{\mathcal{A}}_{2\ell+1}^t$, respectively. We found the nodes of these rules to be in the interval $[-\delta - 1, \delta + 1]$. Computed results are displayed in Table 27. The table shows that higher accuracy is achieved for the same number of nodes than in Table 26.

Table 27: Example 4.3: Results for the last integral in (50).

ℓ	$\mathcal{I}(f) - \mathcal{G}_\ell^t(f)$	$\mathcal{I}(f) - \mathcal{G}_{\ell+2}^t(f)$	$\mathcal{I}(f) - \tilde{\mathcal{A}}_{2\ell+1}^t(f)$	$\mathcal{I}(f) - \tilde{\mathcal{A}}_{2\ell+1}^t(f)$
25	4.933(-6)	-9.210(-6)	2.921(-8)	1.638(-7)
50	2.714(-8)	-4.179(-8)	-1.069(-10)	6.458(-11)
75	3.728(-10)	-4.964(-10)	1.210(-13)	-1.489(-12)
100	8.461(-12)	-9.666(-12)	-7.623(-15)	2.020(-15)

5. Conclusion and extension

This paper investigates the use of the difference between the averaged rules and the associated Gauss rule as an estimate of the quadrature error of the latter. Computed examples illustrate that the accuracy of the averaged rules can be significantly higher than what the degree of exactness of these rules suggests. This property makes the averaged rules useful for estimating the error in Gauss rules. Their application to the estimation of the error of approximations of certain matrix functionals has recently been described in [13]. The results of the present paper shed light on the good performance of averaged rules in this application. Several modifications of the averaged rule that forces them to be interior are discussed.

Acknowledgments

The authors would like to thank Nick Trefethen and the referees for comments. Research by L. Reichel is supported in part by NSF grant DMS-1729509. The research of M. M. Spalević is 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.

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