

Radau- and Lobatto-type averaged Gauss rules

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Abstract

We describe numerical methods for the construction of interpolatory quadrature rules of Radau and Lobatto types. In particular, we are interested in deriving efficient algorithms for computing optimal averaged Gauss-Radau and Gauss-Lobatto type quadrature rules. These averaged rules allow us to estimate the quadrature error in Gauss-Radau and Gauss-Lobatto quadrature rules. This is important since the latter rules have higher algebraic degree of exactness than the corresponding Gauss rules, and this makes it possible to construct averaged quadrature rules of higher algebraic degree of exactness than the corresponding “standard” averaged Gauss rules available in the literature.

Keywords: Gauss quadrature rules, optimal averaged Gauss quadrature rules, anti-Gauss quadrature rules, Gauss-Radau rules, Gauss-Lobatto rules method

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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

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form

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

Gauss quadrature rules are useful for this purpose. The nodes and weights of the ℓ -node Gauss rule associated with the measure $d\omega$,

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

are such that the rule has degree of exactness $2\ell - 1$, i.e.,

$$\mathcal{G}_\ell(f) = \mathcal{I}(f) \quad \forall f \in \mathbb{P}_{2\ell-1}, \quad (3)$$

where $\mathbb{P}_{2\ell-1}$ denotes the set of all polynomials of degree at most $2\ell - 1$. The requirement (3) determines the nodes x_k and weights w_k uniquely. The nodes are known to be distinct and to live in the convex hull of the support of $d\omega$, and the weights w_k are known to be positive; see, e.g., Gautschi [11] for a thorough discussion of Gauss quadrature.

The Gauss rule (2) can be associated with the symmetric tridiagonal matrix

$$T_\ell = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & 0 \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & \\ & \ddots & \ddots & \ddots & \\ 0 & & \sqrt{\beta_{\ell-2}} & \alpha_{\ell-2} & \sqrt{\beta_{\ell-1}} \\ & & & \sqrt{\beta_{\ell-1}} & \alpha_{\ell-1} \end{bmatrix} \in \mathbb{R}^{\ell \times \ell}, \quad (4)$$

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

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

i.e.,

$$p_{k+1}(x) = (x - \alpha_k)p_k(x) - \beta_k p_{k-1}(x), \quad k = 0, 1, \dots, \quad (5)$$

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

$$\alpha_k := \frac{(xp_k, p_k)}{(p_k, p_k)}, \quad \beta_k := \frac{(p_k, p_k)}{(p_{k-1}, p_{k-1})}. \quad (6)$$

Specifically, the nodes and weights of the Gauss rule (2) are the eigenvalues and the squares of the first component of suitably normalized eigenvectors of

the matrix (4), respectively; the nodes and weights can be computed fairly efficiently by the Golub-Welsch algorithm [11, 15]. The recursion coefficients (6) are explicitly known for many classical measures $d\omega(x)$; if they are not known, then they can be conveniently computed for increasing indices by the Stieltjes procedure; see Gautschi [11], Cvetković and Milovanović [4], both for formulas for the α_k and β_k for various measures, and for a discussion of the Stieltjes procedure.

Let for the moment the convex hull of the support of the measure be a bounded interval $[a, b]$. Then it is sometimes convenient to require that the quadrature rule has a node $x'_0 = a$. The requirement that the nodes and weights of an $(\ell + 1)$ -node quadrature rule for the approximation of the integral (1) with the fixed node $x'_0 = a$ be of as high degree of exactness as possible leads to Gauss-Radau rules. It is well-known that the “free” nodes x'_1, \dots, x'_ℓ of the $(\ell + 1)$ -node Gauss-Radau rule are the nodes x_1, \dots, x_ℓ of an ℓ -node Gauss rule associated with the measure $(x - a)d\omega(x)$; see, e.g., [11, p. 25] or [14].

It is also possible to fix two nodes $x'_0 = a$ and $x'_{\ell+1} = b$ of an $(\ell + 2)$ -node quadrature rule. The requirement that the nodes and weights of such an $(\ell + 2)$ -node quadrature rule for the approximation of the integral (1) be of as high degree of exactness as possible leads to Gauss-Lobatto rules. The “free” nodes x'_1, \dots, x'_ℓ of an $(\ell + 2)$ -node Gauss-Lobatto rules are the nodes x_1, \dots, x_ℓ of an ℓ -node Gauss rule associated with the measure $(x - a)(b - x)d\omega(x)$; see [11].

It is the purpose of the present paper to introduce averaged Gauss-Radau and Gauss-Lobatto rules that are analogues of the optimal averaged Gauss rules proposed in [21]. The averaged rules allow us to determine accurate estimates for the error in the underlying Gauss-Radau and Gauss-Lobatto rules. Both “standard” Gauss-Radau and Gauss-Lobatto rules in which the node a and b are of multiplicity one and generalized Gauss-Radau and Gauss-Lobatto rules that allow these nodes to have higher multiplicities are considered; see, e.g., [1, 10, 12, 18] for discussions of generalized Gauss-Radau and Gauss-Lobatto quadrature rules.

This paper is organized as follows. Section 2 discusses the computation of Radau and Lobatto rules (not necessarily Gaussian) with simple or multiple nodes at $x = a$ and $x = b$. Modified anti-Gauss rules, weighted averaged Gauss-Radau and Gauss-Lobatto rules are considered in Section 3. Numerical examples that illustrate the application of the latter rules to the estimation of the quadrature error are presented in Section 4. Concluding remarks can be found in Section 5.

2. Interpolatory quadrature rules of Gauss-Radau and Gauss-Lobatto types

This section discusses the computation of interpolatory quadrature rules of Gauss-Radau and Gauss-Lobatto types. Their construction uses the recursion coefficients (6), but first we describe how to construct Radau and Lobatto extensions of arbitrary interpolatory quadrature rules.

Let the measure $d\lambda$ be nonnegative with infinitely many points of support on the real axis, and such that all moments $\nu_k = \int x^k d\lambda$, $k = 0, 1, \dots$, exist. We can approximate integrals of the form

$$\mathcal{J}(g) = \int g(x) d\lambda(x) \quad (7)$$

by an interpolatory quadrature rule \mathcal{Q}_m with m nodes,

$$\mathcal{Q}_m(g) = \sum_{k=1}^m g(x_k) \lambda_k. \quad (8)$$

We require the nodes x_k to be real and distinct, and to live in the open interval, whose closure is the convex hull of the support of $d\lambda(x)$, which in our case is $[a, b]$, i.e.,

$$a < x_1 < x_2 < \dots < x_m < b. \quad (9)$$

The weights λ_k can be determined so the rule $\mathcal{Q}_m(g)$ has degree of exactness $m - 1$, i.e.,

$$\mathcal{Q}_m(g) = \mathcal{J}(g) \quad \forall f \in \mathbb{P}_{m-1}. \quad (10)$$

The weights λ_k are real numbers.

2.1. Interpolatory quadrature rules of Radau-type with a simple endpoint node

The Radau-type interpolatory quadrature rule associated with the measure $d\omega(x)$ with a node at $x = a$ for approximating the integral (1) is of the form

$$\mathcal{Q}_{m,a}(f) = w_0 f(a) + \sum_{k=1}^m f(x_{k,a}) w_k, \quad (11)$$

where

$$a < x_{1,a} < x_{2,a} < \dots < x_{m,a} < b, \quad (12)$$

and

$$\mathcal{Q}_{m,a}(f) = \mathcal{I}(f) \quad \forall f \in \mathbb{P}_m.$$

Suppose that we know how to calculate the nodes and weights of the rule (8). Substituting $f(x) = (x - a)g(x)$, $g \in \mathbb{P}_{m-1}$, into (1) and (11), letting $d\lambda(x) = (x - a)d\omega(x)$ in (7), comparing (8) and (11), and finally substituting $f(x) \equiv 1$ into (11), we obtain the following formulas for the nodes and coefficients for the quadrature rule (11):

$$\begin{aligned} x_{k,a} &= x_k, \quad k = 1, 2, \dots, m, \\ w_k &= \frac{\lambda_k}{x_{k,a} - a}, \quad k = 1, 2, \dots, m, \\ w_0 &= \mu_0 - \sum_{k=1}^m w_k. \end{aligned} \tag{13}$$

We remark that Radau-type quadrature rules with a node at the endpoint b instead of at the endpoint a can be computed similarly.

2.2. Interpolatory quadrature rules of Radau-type with multiple endpoint nodes

Consider Radau-type quadrature rules associated with the measure $d\omega(x)$ with an endpoint node at a of multiplicity $p \in \mathbb{N}$ for the approximation of the integral (1). These rules are of the form

$$\mathcal{Q}_{m,a}^{(p)}(f) = \sum_{i=0}^{p-1} \eta_i f^{(i)}(a) + \sum_{k=1}^m f(x_{k,a}^{(p)}) w_k, \tag{14}$$

where

$$a < x_{1,a}^{(p)} < x_{2,a}^{(p)} < \dots < x_{m,a}^{(p)} < b, \tag{15}$$

and

$$\mathcal{Q}_{m,a}^{(p)}(f) = \mathcal{I}(f) \quad \forall f \in \mathbb{P}_{m+p-1}.$$

Assume that we know how to compute the nodes and weights of the rule (8). Substituting $f(x) = (x - a)^p g(x)$ into (1) and (14), letting $d\lambda(x) = (x - a)^p d\omega(x)$, and then comparing (8) and (14), gives formulas for calculating the internal nodes and corresponding weights of the rule (14):

$$\begin{aligned} x_{k,a}^{(p)} &= x_k, \quad k = 1, 2, \dots, m, \\ w_k &= \frac{\lambda_k}{(x_{k,a}^{(p)} - a)^p}, \quad k = 1, 2, \dots, m. \end{aligned} \tag{16}$$

We describe two approaches to computing the coefficients η_i , $i = 0, \dots, p-1$, of the quadrature rule (14).

2.2.1. *The first approach to computing the coefficients η_i of (14)*

Let $f(x) \equiv 1$ in (14). Then we obtain

$$\eta_0 = \mu_0 - \sum_{k=0}^m w_k. \quad (17)$$

The coefficients η_i , $i = 1, 2, \dots, p-1$, in (14) can be evaluated consecutively by letting $f(x) = x^i$, $i = 1, 2, \dots, p-1$. This yields the formulas

$$\eta_i = \frac{1}{i!} \left[\mu_i - \sum_{j=0}^{i-1} \frac{i!}{(i-j)!} \eta_j a^{i-j} - \sum_{k=1}^m x_k^i w_k \right], \quad (18)$$

for $i = 1, 2, \dots, p-1$; η_0 is given by (17).

2.2.2. *The second approach to computing the coefficients η_i of (14)*

The measure $d\lambda(x) = (x-a)^p d\omega(x)$ is relevant for computing the internal nodes and associated weights of the rule (14). It can be determined by p successive modifications of the measure $d\omega(x)$ by the linear factor $t-a$; cf. [11, §2.4.2]. This can be accomplished by p applications of the MATLAB function `chri1.m` in [13]. We suppose that we know how to calculate the nodes and weights of the rule (8). For the computation of the nodes x_k and weights λ_k in (8), when this is a Gauss quadrature rule, one can apply the MATLAB function `gauss.m` in [13].

To compute the boundary weights η_i , $i = 0, 1, \dots, p-1$, in (14), we use (14) with $f(x) = f_i(x) = (x-a)^{i-1} \pi_m(x)$, $i = 1, \dots, p$, where

$$\pi_m(x) = \prod_{k=1}^m (x - x_k).$$

Since $f \in \mathbb{P}_{m+p-1}$, the quadrature error of the rule (15) is zero, and all terms in the quadrature sum vanish except for the boundary terms η_j for $j \geq i-1$. Therefore, for $i = 1, 2, \dots, p$,

$$\sum_{j=i-1}^{p-1} \eta_j [(x-a)^{i-1} \pi_m(x)]_{x=a}^{(j)} = b_i, \quad b_i = \int_a^b (x-a)^{i-1} \pi_m(x) d\omega(x). \quad (19)$$

Note that the integrals on the right are computable exactly, except for the influence of round-off errors, by an $\lfloor (p+m+1)/2 \rfloor$ -node Gauss quadrature rule for the measure $d\omega(x)$, where $\lfloor \cdot \rfloor$ denotes the integer part function. After substitutions $j_1 = j+1$, $j = j_1$, we have that for $j = i, i+1, \dots, p$ and

$i = 1, 2, \dots, p$, the equations (19) yield a linear system of algebraic equations with an upper triangular matrix,

$$\mathbf{A}\mathbf{t} = \mathbf{b}, \quad \mathbf{A} \in \mathbb{R}^{p \times p}, \quad \mathbf{t}, \mathbf{b} \in \mathbb{R}^p, \quad (20)$$

where

$$\begin{aligned} \mathbf{A} &= [a_{ij}], \quad a_{ij} = [(x-a)^{i-1} \pi_m(x)]_{x=a}^{(j-1)}, \quad j \geq i; \quad a_{ij} = 0, \quad j < i, \\ \mathbf{t} &= [t_j], \quad t_j = \eta_{j-1}; \quad \mathbf{b} = [b_i]. \end{aligned} \quad (21)$$

Therefore, we can calculate the a_{ij} , for $i = 1, 2, \dots, p$ and $j = i, i+1, \dots, p$ as follows: When $j = i$, we obtain by using Leibnitz's formula

$$\begin{aligned} a_{ii} &= \sum_{j=0}^{i-1} \binom{i-1}{j} \pi_m^{(i-j-1)}(a) [(x-a)^{i-1}]_{x=a}^{(j)} \\ &= (i-1)! \pi_m(a) = (-1)^m (i-1)! \prod_{k=1}^m (a-x_k), \end{aligned} \quad (22)$$

for $i = 1, 2, \dots, p$. For $j > i$, similarly we have

$$\begin{aligned} a_{ij} &= \sum_{k=0}^{j-1} \binom{j-1}{k} \pi_m^{(j-k-1)}(a) [(x-a)^{i-1}]_{x=a}^{(k)} \\ &= (i-1)! \binom{j-1}{i-1} \pi_m^{(j-i)}(a) = \frac{(j-1)!}{(j-i)!} \pi_m^{(j-i)}(a). \end{aligned} \quad (23)$$

Observe that (23) for $j = i$ reduces to (22).

It remains to discuss the computation of $\pi_m^{(j-i)}(a)$. We use the following approach. Consider the calculation of $\pi_m^{(s)}(a)$, $s \in \mathbb{N}$. First we determine $\pi_m^{(s)}(x)$, $s \in \mathbb{N}$ for $x \in (a, x_1)$, and then let $x \rightarrow a+$. We obtain

$$\pi_m(x) = \prod_{k=1}^m (x-x_k) = (-1)^m \prod_{k=1}^m (x_k-x) = (-1)^m e^{y(x)}, \quad (24)$$

where

$$y(x) = \ln \prod_{k=1}^m (x_k-x) = \sum_{k=1}^m \ln(x_k-x). \quad (25)$$

Further, from (24) we obtain

$$\begin{aligned} \pi_m^{(s)}(x) &= (-1)^m (e^{y(x)})^{(s)} = (-1)^m \left(y' \cdot e^{y(x)} \right)^{(s-1)} \\ &= (-1)^m \sum_{\ell=0}^{s-1} \binom{s-1}{\ell} \left(e^{y(x)} \right)^{(s-\ell-1)} y^{(\ell+1)}(x) \end{aligned}$$

and

$$\pi_m^{(s)}(a) = (-1)^m \sum_{\ell=0}^{s-1} \binom{s-1}{\ell} \left(e^{y(x)} \right)_{x=a}^{(s-\ell-1)} y^{(\ell+1)}(a). \quad (26)$$

Finally, differentiation of (25) yields

$$y(a) = \sum_{k=1}^m \ln(x_k - a), \quad y^{(\ell+1)}(a) = - \sum_{k=1}^m \frac{\ell!}{(x_k - a)^{\ell+1}},$$

for $\ell = 0, 1, \dots$. This completes the calculation of (26). We can determine Radau-type formulas with the endpoint node at b of multiplicity $p \in \mathbb{N}$ in an analogous fashion.

2.3. Interpolatory quadrature rules of Lobatto-type with simple endpoints

We consider Lobatto-type formulas with endpoint nodes $a < b$. The $(m+2)$ -node Lobatto-type interpolatory quadrature rule for approximating the integral (1) is of the form

$$\mathcal{Q}_{m,a,b}(f) = w_0 f(a) + \sum_{k=1}^m f(x_{k,a,b}) w_k + w_{m+1} f(b), \quad (27)$$

where

$$a < x_{1,a,b} < x_{2,a,b} < \dots < x_{m,a,b} < b, \quad (28)$$

and

$$\mathcal{Q}_{m,a,b}(f) = \mathcal{I}(f) \quad \forall f \in \mathbb{P}_{m+1}.$$

Assume that we can evaluate the rule (8). Substituting

$$f(x) = (x-a)(b-x)g(x)$$

into (1) and (27), letting $d\lambda(x) = (x-a)(b-x)d\omega(x)$, then comparing (8) and (27), and substituting $f(x) = x-b$ into (27) and $f(x) = x-a$ into (27), we obtain formulas for calculating the nodes and coefficients of (27):

$$\begin{aligned} x_{k,a,b} &= x_k, \quad k = 1, 2, \dots, m, \\ w_k &= \frac{\lambda_k}{(x_{k,a,b} - a)(b - x_{k,a,b})}, \quad k = 1, 2, \dots, m, \\ w_0 &= \frac{1}{b-a} \left[b\mu_0 - \mu_1 + \sum_{k=1}^m w_k (x_{k,a,b} - b) \right], \\ w_{m+1} &= \frac{1}{b-a} \left[\mu_1 - a\mu_0 - \sum_{k=1}^m w_k (x_{k,a,b} - a) \right]. \end{aligned} \quad (29)$$

2.4. *Interpolatory quadrature rules of Lobatto-type with multiple endpoints*

We consider Lobatto-type formulas with endpoint nodes at a and b of multiplicities p and q , $p, q \in \mathbb{N}$, respectively. These rules, associated with the measure $d\omega(x)$ and designed for approximating the integral (1), are of the form

$$\mathcal{Q}_{m,a,b}^{(p,q)}(f) = \sum_{i=0}^{p-1} \eta_i f^{(i)}(a) + \sum_{k=1}^m f(x_{k,a,b}^{(p,q)}) w_k + \sum_{i=0}^{q-1} \zeta_i f^{(i)}(b), \quad (30)$$

where

$$a < x_{1,a,b}^{(p,q)} < x_{2,a,b}^{(p,q)} < \dots < x_{m,a,b}^{(p,q)} < b \quad (31)$$

and

$$\mathcal{Q}_{m,a,b}^{(p,q)}(f) = \mathcal{I}(f) \quad \forall f \in \mathbb{P}_{m+p+q-1}.$$

Suppose that we know how to calculate the rule (8). Letting

$$f(x) = (x - a)^p (b - x)^q g(x)$$

in (1) and (30), using the measure $d\lambda(x) = (x - a)^p (b - x)^q d\omega(x)$, and then comparing (8) and (30), we obtain formulas for calculating the internal nodes and corresponding weights in (30):

$$\begin{aligned} x_{k,a,b}^{(p,q)} &= x_k, \quad k = 1, 2, \dots, m, \\ w_k &= \frac{\lambda_k}{(x_{k,a,b}^{(p,q)} - a)^p (b - x_{k,a,b}^{(p,q)})^q}, \quad k = 1, 2, \dots, m. \end{aligned} \quad (32)$$

We turn to the coefficients η_i , $i = 0, 1, \dots, p-1$, and ζ_i , $i = 0, 1, \dots, q-1$, of (30). The measure

$$d\lambda(x) = (x - a)^p (b - x)^q d\omega(x), \quad (33)$$

which determines the internal nodes and the associated weights can be obtained by $p + q$ consecutive modifications of the measure $d\omega(x)$, p of them with the shift a and q of them with the shift b ; cf. [11, § 2.4.2]. This can be accomplished by $p + q$ applications of the MATLAB function `chri1.m`. We suppose that we know how to calculate the nodes and weights of the rule (8). For the computation of the nodes x_k and weights λ_k in (8), when this is a Gauss quadrature rule, one can use the MATLAB function `gauss.m` in [13].

To evaluate the boundary weights η_i , $i = 0, 1, \dots, p-1$, in (30), we use (30) with $f(x) = f_i(x) = (x-a)^{i-1}\pi_m(x)(b-x)^q$, $i = 1, 2, \dots, p$, where

$$\pi_m(x) = \prod_{k=1}^m (x - x_k).$$

Since $f \in \mathbb{P}_{m+p+q-1}$, the remainder vanishes, and by the choice of f all terms in the quadrature sum are zero except for the boundary terms η_j with $j \geq i-1$. Therefore, for $i = 1, 2, \dots, p$, we have

$$\begin{aligned} \sum_{j=i-1}^{p-1} \eta_j [(x-a)^{i-1}\pi_m(x)(b-x)^q]_{x=a}^{(j)} &= b_i, \\ b_i &= \int_a^b (x-a)^{i-1}\pi_m(x)(b-x)^q d\omega(x). \end{aligned} \quad (34)$$

The integrals above are computable by a $\lfloor (p+q+m+1)/2 \rfloor$ -point Gauss quadrature rule associated with the measure $d\omega(x)$. After the substitutions $j_1 = j+1$, $j = j_1$, we have that for $j = i, i+1, \dots, p$ and $i = 1, 2, \dots, p$ the equations (34) determine a linear system of algebraic equations with an upper triangular matrix

$$\mathbf{A}\mathbf{t} = \mathbf{b}, \quad \mathbf{A} \in \mathbb{R}^{p \times p}, \quad \mathbf{t}, \mathbf{b} \in \mathbb{R}^p, \quad (35)$$

where

$$\begin{aligned} \mathbf{A} &= [a_{ij}], \quad a_{ij} = [(x-a)^{i-1}\pi_m(x)(b-x)^q]_{x=a}^{(j-1)}, \quad j \geq i; \quad a_{ij} = 0, \quad j < i, \\ \mathbf{t} &= [t_j], \quad t_j = \eta_{j-1}; \quad \mathbf{b} = [b_i]. \end{aligned} \quad (36)$$

We have to calculate the a_{ij} for $j = i, i+1, \dots, p$ and $i = 1, 2, \dots, p$. This can be achieved as follows: When $j = i$, we have by Leibnitz's formula

$$\begin{aligned} a_{ii} &= \sum_{j=0}^{i-1} \binom{i-1}{j} \Pi_{m,q}^{(i-j-1)}(a) [(x-a)^{i-1}]_{x=a}^{(j)} \\ &= (i-1)! \Pi_{m,q}(a) = (-1)^m (i-1)! \prod_{k=1}^m (a-x_k)(b-a)^q, \end{aligned} \quad (37)$$

for $i = 1, 2, \dots, p$, where

$$\Pi_{m,q}(x) = \pi_m(x)(b-x)^q.$$

When $j > i$, we again use Leibnitz's formula to obtain

$$\begin{aligned} a_{ij} &= \sum_{k=0}^{j-1} \binom{j-1}{k} \Pi_{m,q}^{(j-k-1)}(a) [(x-a)^{i-1}]_{x=a}^{(k)} \\ &= (i-1)! \binom{j-1}{i-1} \Pi_{m,q}^{(j-i)}(a) = \frac{(j-1)!}{(j-i)!} \Pi_{m,q}^{(j-i)}(a). \end{aligned} \quad (38)$$

Observe that for $j = i$ (38) gives (37).

It remains to discuss the evaluation of $\Pi_{m,q}^{(j-i)}(a)$. Consider the calculation of $\Pi_{m,q}^{(s)}(a)$, $s \in \mathbb{N}$. We first determine $\Pi_{m,q}^{(s)}(x)$ for $s \in \mathbb{N}$ for $x \in (a, x_1)$, and then let $x \rightarrow a+$. This yields

$$\Pi_{m,q}(x) = \prod_{k=1}^m (x - x_k)(b - x)^q = (-1)^m \prod_{k=1}^m (x_k - x)(b - x)^q = (-1)^m e^{y(x)}, \quad (39)$$

where

$$y(x) = \ln \prod_{k=1}^m (x_k - x)(b - x)^q = \sum_{k=1}^m \ln(x_k - x) + q \ln(b - x). \quad (40)$$

Further,

$$\begin{aligned} \Pi_{m,q}^{(s)}(x) &= (-1)^m (e^{y(x)})^{(s)} = (-1)^m \left(y' \cdot e^{y(x)} \right)^{(s-1)} \\ &= (-1)^m \sum_{\ell=0}^{s-1} \binom{s-1}{\ell} \left(e^{y(x)} \right)^{(s-\ell-1)} y^{(\ell+1)}(x) \end{aligned}$$

and

$$\Pi_{m,q}^{(s)}(a) = (-1)^m \sum_{\ell=0}^{s-1} \binom{s-1}{\ell} \left(e^{y(x)} \right)_{x=a}^{(s-\ell-1)} y^{(\ell+1)}(a). \quad (41)$$

Differentiating (40) gives

$$\begin{aligned} y(a) &= \sum_{k=1}^m \ln(x_k - a) + q \ln(b - a), \\ y^{(\ell+1)}(a) &= - \sum_{k=1}^m \frac{\ell!}{(x_k - a)^{\ell+1}} - q \frac{\ell!}{(b - a)^{\ell+1}}, \end{aligned}$$

for $\ell = 0, 1, \dots$. This completes the calculation of (41).

To evaluate the boundary weights ζ_i , $i = 0, 1, \dots, q-1$, in (30), we use (30) with

$$f(x) = f_i(x) = (x-b)^{i-1}(-1)^q \pi_m(x)(x-a)^p, \quad i = 1, 2, \dots, q,$$

where $\pi_m(x) = \prod_{k=1}^m (x-x_k)$. Since $f \in \mathbb{P}_{m+p+q-1}$, the remainder in the quadrature rule vanishes and all terms in the quadrature sum are zero except for the boundary terms ζ_j for $j \geq i-1$. Therefore, for $i = 1, 2, \dots, q$, we obtain

$$\begin{aligned} \sum_{j=i-1}^{q-1} \zeta_j [(x-b)^{i-1}(-1)^q \pi_m(x)(x-a)^p]_{x=b}^{(j)} &= b_i, \\ b_i &= \int_a^b (x-b)^{i-1}(-1)^q \pi_m(x)(x-a)^p d\omega(x). \end{aligned} \quad (42)$$

The above integrals can be computed exactly (up to round-off errors) by a $\lfloor (p+q+m+1)/2 \rfloor$ -node Gauss quadrature rule associated with the measure $d\omega(x)$. Letting $j_1 = j+1$, $j = j_1$, and substituting for $j = i, i+1, \dots, q$ and $i = 1, 2, \dots, q$ these equations into (34) yield a linear system of equations with an upper triangular matrix,

$$\mathbf{A}\mathbf{t} = \mathbf{b}, \quad \mathbf{A} \in \mathbb{R}^{q \times q}, \quad \mathbf{t}, \mathbf{b} \in \mathbb{R}^q, \quad (43)$$

where

$$\begin{aligned} \mathbf{A} &= [a_{ij}], \quad a_{ij} = [(x-b)^{i-1}(-1)^q \pi_m(x)(x-a)^p]_{x=b}^{(j-1)}, \quad j \geq i; \quad a_{ij} = 0, \quad j < i, \\ \mathbf{t} &= [t_j], \quad t_j = \zeta_{j-1}; \quad \mathbf{b} = [b_i]. \end{aligned} \quad (44)$$

We have to calculate the coefficients a_{ij} for $j = i, i+1, \dots, q$ and $i = 1, 2, \dots, q$. When $j = i$, we obtain similarly as above

$$\begin{aligned} a_{ii} &= \sum_{j=0}^{i-1} \binom{i-1}{j} \Pi_{m,p}^{(i-j-1)}(b) [(x-b)^{i-1}]_{x=b}^{(j)} \\ &= (i-1)! \Pi_{m,p}(b) = (-1)^q (i-1)! \prod_{k=1}^m (b-x_k)(b-a)^p, \end{aligned} \quad (45)$$

for $i = 1, 2, \dots, q$, where

$$\Pi_{m,p}(x) = (-1)^q \pi_m(x)(x-a)^p.$$

For $j > i$, similarly we have

$$\begin{aligned} a_{ij} &= \sum_{k=0}^{j-1} \binom{j-1}{k} \Pi_{m,p}^{(j-k-1)}(b) [(x-b)^{i-1}]_{x=b}^{(k)} \\ &= (i-1)! \binom{j-1}{i-1} \Pi_{m,p}^{(j-i)}(a) = \frac{(j-1)!}{(j-i)!} \Pi_{m,p}^{(j-i)}(b). \end{aligned} \quad (46)$$

It remains to discuss how to compute $\Pi_{m,p}^{(j-i)}(b)$. We use the following approach: Consider the calculation of $\Pi_{m,p}^{(s)}(b)$, $s \in \mathbb{N}$. First we determine $\Pi_{m,p}^{(s)}(x)$, $s \in \mathbb{N}$, for $x \in (x_m, b)$, and then let $x \rightarrow b^-$. This yields

$$\Pi_{m,p}(x) = (-1)^q \prod_{k=1}^m (x - x_k)(x - a)^p = (-1)^q e^{y(x)}, \quad (47)$$

where

$$y(x) = \ln \prod_{k=1}^m (x - x_k)(x - a)^p = \sum_{k=1}^m \ln(x - x_k) + p \ln(x - a). \quad (48)$$

Furthermore,

$$\begin{aligned} \Pi_{m,p}^{(s)}(x) &= (-1)^q (e^{y(x)})^{(s)} = (-1)^q \left(y' \cdot e^{y(x)} \right)^{(s-1)} \\ &= (-1)^q \sum_{\ell=0}^{s-1} \binom{s-1}{\ell} \left(e^{y(x)} \right)^{(s-\ell-1)} y^{(\ell+1)}(x) \end{aligned}$$

and

$$\Pi_{m,p}^{(s)}(b) = (-1)^q \sum_{\ell=0}^{s-1} \binom{s-1}{\ell} \left(e^{y(x)} \right)_{x=b}^{(s-\ell-1)} y^{(\ell+1)}(b). \quad (49)$$

We obtain by differentiating (48),

$$\begin{aligned} y(b) &= \sum_{k=1}^m \ln(b - x_k) + p \ln(b - a), \\ y^{(\ell+1)}(b) &= \sum_{k=1}^m \frac{(-1)^\ell \ell!}{(b - x_k)^{\ell+1}} + p \frac{(-1)^\ell \ell!}{(b - a)^{\ell+1}}, \end{aligned}$$

for $\ell = 0, 1, \dots$. This completes the evaluation of (49).

3. Modified anti-Gauss and weighted averaged Gauss quadrature rules of Radau and Lobatto types

We consider the computation of modified anti-Gauss and weighted averaged Gauss quadrature rules of Radau and Lobatto type with one or two preassigned nodes, respectively. In particular, we consider a sub-class of these rules, that are optimal in the sense of having maximal degree of exactness. For more details on generalized averaged Gauss quadrature rules and their numerical computation; see [20] as well as [9, 16, 19, 21].

An ℓ -node Gauss quadrature rule of Lobatto-type for the approximation of the integral (1) with fixed nodes at $x = a$ and $x = b$ of multiplicities p and q , respectively, is a formula of the form

$$\tilde{\mathcal{G}}_\ell^{p,q}(f) = \sum_{j=0}^{p-1} \tilde{\eta}_j f^{(j)}(a) + \sum_{k=0}^{\ell} f(\tilde{x}_k) \tilde{w}_k + \sum_{j=0}^{q-1} \tilde{\zeta}_j f^{(j)}(b), \quad (50)$$

whose nodes and weights are chosen so that

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

An $(\ell + 1)$ -node modified anti-Gauss quadrature rule of Lobatto-type for approximating the integral (1) with fixed nodes at $x = a$ and $x = b$ of multiplicities p and q , respectively, which corresponds to the Gauss quadrature rule (50), is a formula of the form

$$\hat{\mathcal{A}}_{\ell+1}^{p,q}(f) = \sum_{j=0}^{p-1} \hat{\eta}_j f^{(j)}(a) + \sum_{k=0}^{\ell+1} f(\hat{x}_k) \hat{w}_k + \sum_{j=0}^{q-1} \hat{\zeta}_j f^{(j)}(b), \quad (51)$$

whose nodes and weights are chosen so that

$$\hat{\mathcal{A}}_{\ell+1}^{p,q}(f) = \mathcal{I}(f) \quad \forall f \in \mathbb{P}_{2\ell+p+q-1}.$$

An $(2\ell + 1)$ -node weighted averaged Gauss quadrature rule of Lobatto-type for approximating the integral (1) with fixed nodes at $x = a$ and $x = b$ of multiplicities p and q , respectively, which corresponds to the Gauss quadrature rule (50), is a formula of the form

$$\check{\mathcal{S}}_{2\ell+1}^{p,q}(f) = \sum_{j=0}^{p-1} \check{\eta}_j f^{(j)}(a) + \sum_{k=0}^{2\ell+1} f(\check{x}_k) \check{w}_k + \sum_{j=0}^{q-1} \check{\zeta}_j f^{(j)}(b), \quad (52)$$

whose nodes and weights are chosen so that

$$\check{\mathcal{S}}_{2\ell+1}^{p,q}(f) = \mathcal{I}(f) \quad \forall f \in \mathbb{P}_{2\ell+p+q+1}.$$

In the case when $\check{\mathcal{S}}_{2\ell+1}^{p,q}(f)$ is an $(2\ell+1)$ -point optimal generalized averaged Gauss quadrature rule of Lobatto-type for the integral (1) with fixed nodes at $x = a$ and $x = b$ of multiplicities p and q , respectively, which corresponds to the Gaussian quadrature rule (50); cf. [21, 19], then

$$\check{\mathcal{S}}_{2\ell+1}^{p,q}(f) = \mathcal{I}(f) \quad \forall f \in \mathbb{P}_{2\ell+p+q+2}.$$

If $q = 0$ in the quadrature rules (50), (51), and (52), then we obtain Radau-type quadrature rules. If in addition $p = 1$, then the Radau rules have a simple node at $x = a$. If differentiation of f is complicated, then it may be attractive to use quadrature rules of Radau or Lobatto-types with simple nodes at a or b .

By substituting

$$f(x) = (x - a)^p(b - x)^q g(x)$$

into (1), we obtain $\mathcal{I}(f) = \mathcal{J}(g)$, where $\mathcal{J}(g)$ is given by (7) and the new measure (33). The quadrature rules $\check{\mathcal{G}}_{\ell}^{p,q}(f)$, $\check{\mathcal{A}}_{\ell+1}^{p,q}(f)$, and $\check{\mathcal{S}}_{2\ell+1}^{p,q}(f)$ for approximating the integral (1) are also quadrature rules for the integrand g and measure (33).

Assume that the entries of the matrix T_k , defined by (4), are known. These entries are determined by the recursion coefficients (6) for monic orthogonal polynomials with respect to the measure $d\omega$. Gautschi [11, § 2.4] describes algorithms for determining the symmetric tridiagonal matrix, for suitable values of $\ell \leq k$,

$$T'_{\ell} = \begin{bmatrix} \alpha'_0 & \sqrt{\beta'_1} & & & 0 \\ \sqrt{\beta'_1} & \alpha'_1 & \sqrt{\beta'_2} & & \\ & \ddots & \ddots & \ddots & \\ & & \sqrt{\beta'_{\ell-2}} & \alpha'_{\ell-2} & \sqrt{\beta'_{\ell-1}} \\ 0 & & & \sqrt{\beta'_{\ell-1}} & \alpha'_{\ell-1} \end{bmatrix} \in \mathbb{R}^{\ell \times \ell}, \quad (53)$$

whose entries are determined by the recursion coefficients for monic orthogonal polynomials with respect to the measure (33). The matrix (53) determines an ℓ -node Gauss quadrature rule with respect to the measure (33). An algorithm also is described in [14].

Introduce the reverse matrix

$$T_\ell'' = \begin{bmatrix} \alpha'_{\ell-1} & \sqrt{\beta'_{\ell-1}} & & & & 0 \\ \sqrt{\beta'_{\ell-1}} & \alpha'_{\ell-2} & \sqrt{\beta'_{\ell-2}} & & & \\ & \ddots & \ddots & \ddots & & \\ 0 & & \sqrt{\beta'_2} & \alpha'_1 & \sqrt{\beta'_1} & \\ & & & \sqrt{\beta'_1} & \alpha'_0 & \end{bmatrix} \in \mathbb{R}^{\ell \times \ell}, \quad (54)$$

which is obtained by reversing the order of the rows and columns of the matrix (53). The concatenated matrix

$$T_{2\ell+1}''' = \begin{bmatrix} T_\ell' & \sqrt{\beta'_\ell} e_\ell & 0 \\ \sqrt{\beta'_\ell} e_\ell^T & \alpha'_\ell & \sqrt{\beta'_1} e_1^T \\ 0 & \sqrt{\beta'_1} e_1 & T_\ell'' \end{bmatrix} \in \mathbb{R}^{(2\ell+1) \times (2\ell+1)} \quad (55)$$

is associated with $(2\ell + 1)$ -node weighted averaged Gauss quadrature rules

$$\mathcal{S}_{2\ell+1}(g) = \sum_{k=1}^{2\ell+1} f(x_k) \lambda_k \quad (56)$$

with respect to the measure $d\lambda(x)$. These rules satisfy

$$\mathcal{S}_{2\ell+1}(g) = \mathcal{J}(g) \quad \forall g \in \mathbb{P}_{2\ell+1}; \quad (57)$$

see, e.g., [20, 21] for discussions on weighted averaged Gauss quadrature rules. We remark that equation (57) holds for an arbitrary choice of the coefficient $\beta' > 0$ in (55).

A special case of the rules $\mathcal{S}_{2\ell+1}$ are the averaged Gauss quadrature rules, where $\beta' = \beta'_\ell$ in (55). These rules were introduced by Laurie [16]. Another well-studied special case are the optimal generalized averaged Gauss quadrature rules, for which $\beta' = \beta'_{\ell+1}$ in (55). The latter rules were first considered by Spalević [21]; see also [9, 20, 19, 22] for further results on these rules. The optimal generalized averaged Gauss quadrature rule with $2\ell + 1$ nodes achieve the maximal degree of precision, which is at least $2\ell + 2$. In case the measure $d\lambda(x)$ that defines the rule is symmetric with respect to the origin, the degree of precision is higher; see, e.g., [20] for details.

Assume that the optimal generalized averaged Gauss quadrature rule with respect to the measure (33) with $2\ell + 1$ nodes $x_1 < x_2 < \dots < x_{2\ell+1}$ is internal, i.e., all nodes live in the convex hull of the support of the measure. In case this rule were not internal with either one of the nodes x_1 or $x_{2\ell+1}$

outside the convex hull of the support of (33), then the rule often can be made internal by a suitable choice of β' ; see [20, 7]. The nodes x_k , $k = 1, 2, \dots, 2\ell + 1$, are the “free” nodes of the weighted averaged Gaussian quadrature rule (52) with fixed nodes at $x = a$ and $x = b$. The weights of the rule (52) in the case $p = 1$ and $q = 0$ are given by

$$\check{w}_k = \frac{\lambda_k}{x_k - a}, \quad 1 \leq k \leq 2\ell + 1,$$

$$\check{\eta}_0 = \mu_0 - \sum_{k=1}^{2\ell+1} \check{w}_k,$$

while when $p = q = 1$, we have

$$\check{w}_k = \frac{\lambda_k}{(x_k - a)(b - x_k)}, \quad 1 \leq k \leq 2\ell + 1,$$

$$\check{\eta}_0 = \frac{1}{b - a} \left[b\mu_0 - \mu_1 - \sum_{k=1}^{2\ell+1} \check{w}_k (b - x_k) \right],$$

$$\check{\zeta}_0 = \frac{1}{b - a} \left[\mu_1 - a\mu_0 - \sum_{k=1}^{2\ell+1} \check{w}_k (x_k - a) \right].$$

The last facts easily can be shown similarly as for the corresponding Radau-Kronrod and Lobatto-Kronrod quadrature rules; see [3, 17].

We turn to the anti-Gauss quadrature rules $\widehat{\mathcal{A}}_{\ell+1}^{p,q}(f)$ in (51), which are Lobatto (Radau) modifications of anti-Gauss quadrature rules introduced by Laurie in [16]. Let $\mathcal{A}_{\ell+1}(g)$ denote the $(\ell + 1)$ -node anti-Gauss rule associated with the ℓ -node Gauss rule $\mathcal{G}_\ell(g)$ with respect to the measure (33). The nodes and weights of $\mathcal{A}_{\ell+1}(g)$ can be determined from the symmetric tridiagonal matrix

$$J'_{\ell+1} = \begin{bmatrix} \alpha'_0 & \sqrt{\beta'_1} & & & 0 \\ \sqrt{\beta'_1} & \alpha'_1 & \sqrt{\beta'_2} & & \\ & \ddots & \ddots & \ddots & \\ & & \sqrt{\beta'_{\ell-1}} & \alpha'_{\ell-1} & \sqrt{\beta'_\ell + \beta'} \\ 0 & & & \sqrt{\beta'_\ell + \beta'} & \alpha'_\ell \end{bmatrix} \in \mathbb{R}^{(\ell+1) \times (\ell+1)} \quad (58)$$

with $\beta' = \beta'_\ell$ by the Golub-Welsch algorithm [11, 15]. In general, the value of the parameter $\beta' = \beta'_\ell$ depends on the size of the matrix $J'_{\ell+1}$. In the numerical examples (below) which have been done for the Jacobi weight

functions (68), it is obvious that the parameter β'_ℓ can be easily determined as the corresponding β'_ℓ -coefficient given in [11, Table 1.1, p. 29] for the Jacobi measure (see (33)) $d\lambda(x) = (1-x)^{s+q}(1+x)^{t+p} dx$.

Define the quadrature errors

$$\varepsilon_\ell^G(g) = \mathcal{J}(g) - \mathcal{G}_\ell(g), \quad \varepsilon_{\ell+1}^A(g) = \mathcal{J}(g) - \mathcal{A}_{\ell+1}(g).$$

The nodes and weights of the $(\ell+1)$ -point anti-Gauss rule $\mathcal{A}_{\ell+1}$ are uniquely determined by the requirement

$$\varepsilon_{\ell+1}^A(g) = -\varepsilon_\ell^G(g) \quad \forall g \in \mathbb{P}_{2\ell+1}; \quad (59)$$

see Laurie [16].

Due to the relation (59), an $(\ell+1)$ -node anti-Gauss rule gives for many integrands g a quadrature error of opposite sign as the corresponding ℓ -node Gauss rule. The following theorem shows that a result analogous to (59) also holds for modified ant-Gaussian quadrature rules that are derived from $\mathcal{A}_{\ell+1}(g)$.

Theorem 1. *Let the quadrature rules $\tilde{\mathcal{G}}_\ell^{p,q}(f)$ and $\hat{\mathcal{A}}_{\ell+1}^{p,q}(f)$ be given by (50) and (51), respectively, with $\hat{\mathcal{A}}_{\ell+1}^{p,q}(f)$ determined by the rule $\mathcal{A}_{\ell+1}(g)$. Let*

$$\tilde{\mathcal{E}}_\ell(f) = \mathcal{I}(f) - \tilde{\mathcal{G}}_\ell^{p,q}(f), \quad \hat{\mathcal{E}}_{\ell+1}(f) = \mathcal{I}(f) - \hat{\mathcal{A}}_{\ell+1}^{p,q}(f). \quad (60)$$

Then

$$\hat{\mathcal{E}}_{\ell+1}(f) = -\tilde{\mathcal{E}}_\ell(f) \quad \forall f \in \mathbb{P}_{2\ell+p+q+1}. \quad (61)$$

Proof. First note that

$$(x-a)^p = \sum_{j=0}^p \binom{p}{j} x^{p-j} (-1)^j a^j = x^p - pa x^{p-1} + \pi_{p-2}^{(a)}(x)$$

and

$$\begin{aligned} (b-x)^q &= (-1)^q (x-b)^q = (-1)^q \sum_{j=0}^q \binom{q}{j} x^{q-j} (-1)^j b^j \\ &= (-1)^q x^q - (-1)^q q b x^{q-1} + \pi_{q-2}^{(b)}(x), \end{aligned}$$

where $\pi_{p-2}^{(a)}$ and $\pi_{q-2}^{(b)}$ are polynomials of degrees $p-2$ and $q-2$, respectively. We obtain that

$$(x-a)^p (b-x)^q = (-1)^q x^{p+q} + (-1)^{q-1} (pa+qb) x^{p+q-1} + \pi_{p+q-2}(x), \quad (62)$$

where $\pi_{p+q-2}(x)$ is an algebraic polynomial of degree $p + q - 2$ given by

$$\begin{aligned}\pi_{p+q-2}(x) &= (-1)^q paqb x^{p+q-2} + (x^p - pa x^{p-1}) \pi_{q-2}^{(b)}(x) \\ &\quad + ((-1)^q x^q + (-1)^{q+1} qb x^{q-1} + \pi_{q-2}^{(b)}(x)) \pi_{p-2}^{(a)}(x).\end{aligned}$$

Let f be an arbitrary polynomial of degree $2\ell + p + q + 1$ of the form

$$f(x) = \alpha_{2\ell+p+q+1} x^{2\ell+p+q+1} + \alpha_{2\ell+p+q} x^{2\ell+p+q} + P_{2\ell+p+q-1}(x), \quad (63)$$

where $\alpha_{2\ell+p+q+1}, \alpha_{2\ell+p+q} \in \mathbb{R}$, $P_{2\ell+p+q-1} \in \mathbb{P}_{2\ell+p+q-1}$. Then

$$\widehat{\mathcal{E}}_{\ell+1}(P_{2\ell+p+q-1}) = -\widetilde{\mathcal{E}}_{\ell}(P_{2\ell+p+q-1}) (= 0). \quad (64)$$

Further, it follows from (62) that

$$\begin{aligned}\gamma(x) &= \alpha_{2\ell+p+q+1} x^{2\ell+p+q+1} + \alpha_{2\ell+p+q} x^{2\ell+p+q} \\ &= x^{2\ell+1} (\alpha_{2\ell+p+q+1} x^{p+q} + \alpha_{2\ell+p+q} x^{p+q-1}) \\ &= x^{2\ell+1} ((-1)^q \alpha_{2\ell+p+q+1} (-1)^q x^{p+q} + \alpha_{2\ell+p+q} x^{p+q-1}) \\ &= x^{2\ell+1} \{ (-1)^q \alpha_{2\ell+p+q+1} [(-1)^q x^{p+q} + (-1)^{q-1} (pa + qb) x^{p+q-1}] \\ &\quad + \pi_{p+q-2}(x) - (-1)^{q-1} (pa + qb) x^{p+q-1} - \pi_{p+q-2}(x) \} \\ &\quad + \alpha_{2\ell+p+q} x^{p+q-1} \} \\ &= x^{2\ell+1} \{ (-1)^q \alpha_{2\ell+p+q+1} (x-a)^p (b-x)^q \\ &\quad + (\alpha_{2\ell+p+q+1} (pa + qb) + \alpha_{2\ell+p+q}) x^{p+q-1} \\ &\quad - (-1)^q \alpha_{2\ell+p+q+1} \pi_{p+q-2}(x) \} \\ &= (-1)^q \alpha_{2\ell+p+q+1} x^{2\ell+1} (x-a)^p (b-x)^q \\ &\quad + x^{2\ell} [\alpha_{2\ell+p+q+1} (pa + qb) + \alpha_{2\ell+p+q}] x^{p+q} \\ &\quad + (-1)^{q+1} \alpha_{2\ell+p+q+1} x^{2\ell+1} \pi_{p+q-2}(x) \\ &= h(x) \cdot (x-a)^p (b-x)^q + Q_{2\ell+p+q-1}(x),\end{aligned}$$

where

$$h(x) = (-1)^q \alpha_{2\ell+p+q+1} x^{2\ell+1} + (-1)^q [\alpha_{2\ell+p+q+1} (pa + qb) + \alpha_{2\ell+p+q}] x^{2\ell}$$

and

$$\begin{aligned}Q_{2\ell+p+q-1}(x) &= (-1)^q [\alpha_{2\ell+p+q+1} (pa + qb) + \alpha_{2\ell+p+q}] x^{2\ell} \\ &\quad \times ((-1)^q (pa + qb) x^{p+q-1} - \pi_{p+q-2}(x)) \\ &\quad + (-1)^{q+1} \alpha_{2\ell+p+q+1} x^{2\ell+1} \pi_{p+q-2}(x) \quad (\in \mathbb{P}_{2\ell+p+q-1}).\end{aligned}$$

Let $s(x) = h(x) \cdot (x - a)^p(b - x)^q$. We conclude that

$$\widehat{\mathcal{E}}_{\ell+1}(s) = \varepsilon_{\ell+1}^A(h) = -\varepsilon_{\ell}^G(h) = -\widetilde{\mathcal{E}}_{\ell}(s),$$

i.e.,

$$\widehat{\mathcal{E}}_{\ell+1}(s) = -\widetilde{\mathcal{E}}_{\ell}(s), \quad (65)$$

since $h \in \mathbb{P}_{2\ell+1}$.

It is clear that

$$\widehat{\mathcal{E}}_{\ell+1}(Q_{2\ell+p+q-1}) = -\widetilde{\mathcal{E}}_{\ell}(Q_{2\ell+p+q-1}) (= 0). \quad (66)$$

Since $\gamma(x) = s(x) + Q_{2\ell+p+q-1}(x)$, using the linearity of the operators $\widehat{\mathcal{E}}_{\ell+1}$ and $\widetilde{\mathcal{E}}_{\ell}$, and summing the left and right hand-sides of (65) and (66), we obtain

$$\widehat{\mathcal{E}}_{\ell+1}(\gamma) = -\widetilde{\mathcal{E}}_{\ell}(\gamma). \quad (67)$$

Finally, since $f(x) = \gamma(x) + P_{2\ell+p+q-1}(x)$, summing the left and right hand-sides of (64) and (67), we obtain (61). \square

Remark 1. The modified anti-Gauss quadrature rules $\widehat{\mathcal{A}}_{\ell+1}^{p,q}(f)$ in (51) are Lobatto (Radau) modifications of the modified anti-Gauss quadrature rules considered by Ehrlich [9], as well as in [2]; see also [20]. They can be constructed by applying the Golub-Welsch algorithm [11, 15] to the matrix $J'_{\ell+1}$ in (58) with an arbitrary $\beta' > 0$. Results in this section also hold for these rules, in particular an analog of Theorem 1 is valid.

Remark 2. Similarly as for the quadrature the Lobatto- and Radau-type rules of this paper, it is possible to define Lobatto and Radau extensions of the truncated variants of the optimal generalized Gaussian rules. For the latter rules; see [20] and references therein.

4. Numerical examples

We will use Jacobi weight functions

$$w_{s,t}(x) = (1 - x)^s(1 + x)^t, \quad -1 < x < 1, \quad s > -1, \quad t > -1, \quad (68)$$

for different values of s and t in the computed examples. All computations have been carried out with high-precision arithmetic using 110 to 120 significant decimal digits. This is enough to make round-off errors introduced during the computations negligible.

Table 1: Example 1: Results for the integral (69).

ℓ	$\mathcal{E}_\ell^G(f)$	$\mathcal{E}_{\ell+1}^A(f)$	p, q	$\tilde{\mathcal{E}}_\ell(f)$	$\hat{\mathcal{E}}_{\ell+1}(f)$
5	-6.3497(-7)	6.3889(-7)	1, 0	5.3947(-7)	-5.4087(-7)
10	1.5159(-14)	-1.5169(-14)	1, 0	-5.6156(-15)	5.6179(-15)
20	1.8651(-32)	-1.8652(-32)	1, 0	-2.8381(-33)	2.8383(-33)
30	1.5490(-52)	-1.5490(-52)	1, 0	-1.4386(-53)	1.4386(-53)
40	4.6728(-74)	-4.6729(-74)	1, 0	-3.1002(-75)	3.1003(-75)

Example 1. Consider the integral

$$\mathcal{I}(f) = \int_{-1}^1 f(x) w_{1/2,5}(x) dx, \quad f(x) = \exp(-x^2), \quad (69)$$

whose value is about $\mathcal{I}(f) \approx 3.4574431$. We supply this value to make it possible to assess the relative quadrature error from Table 1. This table shows quadrature errors $\mathcal{E}_\ell^G(f) = \mathcal{I}(f) - \mathcal{G}_\ell(f)$ for the Gauss rules $\mathcal{G}_\ell(f)$, quadrature errors $\mathcal{E}_{\ell+1}^A(f) = \mathcal{I}(f) - \mathcal{A}_{\ell+1}(f)$ for the associated anti-Gauss rules $\mathcal{A}_{\ell+1}(f)$, as well as the quadrature errors (60) for Gauss-Radau rules $\tilde{\mathcal{G}}_\ell^{1,0}(f)$ and associated anti-Gauss rules of Radau-type $\hat{\mathcal{A}}_{\ell+1}^{1,0}(f)$. The latter rules have a fixed node at -1 . The table shows the quadrature errors for the latter quadrature formulas to be slightly smaller than for the former. Note that the errors $\mathcal{E}_\ell^G(f)$ and $\mathcal{E}_{\ell+1}^A(f)$ are of opposite signs and of about the same magnitude. This also holds for the errors $\tilde{\mathcal{E}}_\ell(f)$ and $\hat{\mathcal{E}}_{\ell+1}(f)$. Table 2 shows the corresponding quadrature errors when $p = 0$ and $q = 1$, and the fixed node is at $x = 1$, as well as the quadrature errors when $p = q = 1$ and the fixed nodes are at $x = \pm 1$. Finally, Table 3 display the quadrature errors when $p = 2$, $p = 3$, and $q = 0$, and the fixed node is at $x = -1$.

Example 2. We consider the integral

$$\mathcal{I}(f) = \int_{-1}^1 f(x) w_{0,0}(x) dx, \quad f(x) = \exp(-x^2) \quad (70)$$

with the same integrand f as in Example 1, but with the smooth weight function $w_{0,0}(x) \equiv 1$. Table 4 displays the magnitude of the quadrature errors $\mathcal{E}_\ell(f)$ and $\check{\mathcal{E}}_{2\ell+1}(f) = \mathcal{I}(f) - \check{\mathcal{S}}_{2\ell+1}^{1,0}(f)$, where $\check{\mathcal{S}}_{2\ell+1}^{1,0}(f)$ is the optimal generalized averaged Gauss rule of Radau-type. The table also shows the magnitude of the errors $\mathcal{E}_{2\ell+1}^K(f) = \mathcal{I}(f) - \mathcal{K}_{2\ell+1}^{1,0}(f)$ and the estimates for

Table 2: Example 1: Results for the integral (69).

ℓ	p, q	$\tilde{\mathcal{E}}_\ell(f)$	$\hat{\mathcal{E}}_{\ell+1}(f)$	p, q	$\tilde{\mathcal{E}}_\ell(f)$	$\hat{\mathcal{E}}_{\ell+1}(f)$
5	0, 1	-3.8302(-7)	3.8389(-7)	1, 1	-6.7742(-8)	6.8025(-8)
10	0, 1	4.4657(-15)	-4.4672(-15)	1, 1	6.0309(-16)	-6.0349(-16)
20	0, 1	2.4857(-33)	-2.4858(-33)	1, 1	2.9948(-34)	-2.9950(-34)
30	0, 1	1.3112(-53)	-1.3112(-53)	1, 1	1.5320(-54)	-1.5321(-54)
40	0, 1	2.8871(-75)	-2.8871(-75)	1, 1	3.3272(-76)	-3.3272(-76)

Table 3: Example 1: Results for the integral (69).

ℓ	p, q	$\tilde{\mathcal{E}}_\ell(f)$	$\hat{\mathcal{E}}_{\ell+1}(f)$	p, q	$\tilde{\mathcal{E}}_\ell(f)$	$\hat{\mathcal{E}}_{\ell+1}(f)$
5	2, 0	1.7228(-7)	-1.7304(-7)	3, 0	-3.6807(-8)	3.6886(-8)
10	2, 0	-1.0538(-15)	1.0546(-15)	3, 0	2.1445(-16)	-2.1455(-16)
20	2, 0	-3.9904(-34)	3.9908(-34)	3, 0	4.8340(-35)	-4.8343(-35)
30	2, 0	-1.8528(-54)	1.8528(-54)	3, 0	1.5132(-55)	-1.5132(-55)
40	2, 0	-3.8334(-76)	3.8334(-76)	3, 0	2.3326(-77)	-2.3326(-77)

the error in $\mathcal{G}_\ell^{1,0}(f)$,

$$\check{r}_\ell = \left| \check{\mathcal{S}}_{2\ell+1}^{1,0}(f) - \mathcal{G}_\ell^{1,0}(f) \right|, \quad r_\ell^K = \left| \mathcal{K}_{2\ell+1}^{1,0}(f) - \mathcal{G}_\ell^{1,0}(f) \right|.$$

Here $\mathcal{K}_{2\ell+1}^{1,0}(f)$ denotes the Radau-Kronrod quadrature rule that corresponds to the Gauss-Radau rule $\tilde{\mathcal{G}}_\ell^{1,0}(f)$ with a node at $x = -1$. These kinds of Kronrod rules are discussed in [3, 17]. The exact value of the integral (70) is approximately $\mathcal{I}(f) \approx 1.4936482$. The Radau-Kronrod rule can be seen to be more accurate than the rule $\check{\mathcal{S}}_{2\ell+1}^{1,0}(f)$, but the quality of the error estimates determined by these rules is about the same. We remark that the rules $\check{\mathcal{S}}_{2\ell+1}^{1,0}(f)$ are simpler to evaluate than the rules $\mathcal{K}_{2\ell+1}^{1,0}(f)$.

Example 3. This example is concerned with the integral

$$\mathcal{I}(f) = \int_{-1}^1 f(x) w_{0,0}(x) dx, \quad f(x) = \frac{1}{1 + 25x^2}, \quad (71)$$

with an integrand f with poles at $\pm i/5$ with $i = \sqrt{-1}$. Here $\mathcal{I}(f) \approx$

Table 4: Example 2: Results for the integral (70).

ℓ	$ \mathcal{E}_\ell(f) $	$\check{\mathcal{E}}_{2\ell+1}(f)$	$ \mathcal{E}_{2\ell+1}^K(f) $	\check{r}_ℓ	r_ℓ^K
3	8.3822(-5)	5.3980(-7)	8.5344(-8)	8.4361(-5)	8.3736(-5)
4	8.3029(-6)	1.0965(-8)	1.1136(-10)	3.3138(-6)	3.3030(-6)
5	1.1350(-7)	2.2183(-10)	1.4437(-12)	1.1373(-7)	1.1351(-7)
6	3.4488(-9)	4.3094(-12)	1.5543(-15)	3.4531(-9)	3.4488(-9)

Table 5: Example 3: Results for the integral (71).

ℓ	$\tilde{\mathcal{E}}_\ell(f)$	$\check{\mathcal{E}}_{2\ell+1}(f)$	$ \mathcal{E}_{2\ell+1}^K(f) $	\check{r}_ℓ	r_ℓ^K
10	9.1084(-4)	1.9890(-4)	2.1748(-4)	7.1194(-4)	6.9337(-4)
20	7.0543(-6)	6.3706(-8)	5.6442(-8)	6.9906(-6)	6.9979(-6)
30	8.8925(-8)	1.8812(-11)	4.5815(-11)	8.8944(-8)	8.8880(-8)
40	1.2635(-9)	3.4925(-13)	2.7311(-14)	1.2638(-9)	1.2635(-9)

0.1781477. Table 5 shows the magnitude of the quadrature errors

$$\begin{aligned}\tilde{\mathcal{E}}_\ell(f) &= \mathcal{I}(f) - \tilde{\mathcal{G}}_\ell^{1,0}(f), \\ \check{\mathcal{E}}_{2\ell+1}(f) &= \mathcal{I}(f) - \check{\mathcal{S}}_{2\ell+1}^{1,0}(f), \\ \mathcal{E}_{2\ell+1}^K(f) &= \mathcal{I}(f) - \mathcal{K}_{2\ell+1}^{1,0}(f),\end{aligned}$$

where $\check{\mathcal{S}}_{2\ell+1}^{1,0}(f)$ is the optimal generalized averaged Gauss rule of Radau-type that is associated with the Gauss-Radau rule $\tilde{\mathcal{G}}_\ell^{1,0}(f)$, and $\mathcal{K}_{2\ell+1}^{1,0}(f)$ denotes the Radau-Kronrod quadrature rule that corresponds to this Gauss-Radau rule. The table also displays the estimates

$$\check{r}_\ell = \left| \check{\mathcal{S}}_{2\ell+1}^{1,0}(f) - \tilde{\mathcal{G}}_\ell^{1,0}(f) \right|, \quad r_\ell^K = \left| \mathcal{K}_{2\ell+1}^{1,0}(f) - \tilde{\mathcal{G}}_\ell^{1,0}(f) \right|,$$

for the error in $\tilde{\mathcal{G}}_\ell^{1,0}(f)$. Both these estimates are seen to be accurate. The results for this examples are analogous to those for Example 3, though for the present integral the optimal generalized averaged Gauss rule of Radau-type yields a smaller quadrature error than the corresponding Radau-Kronrod rule for $\ell = 30$.

Example 4. We consider the integral (69) and display in Table 6 the

Table 6: Example 3.4: Results for the integral (69).

ℓ	$\tilde{\mathcal{E}}_\ell(f)$	$\check{\mathcal{E}}_{2\ell+1}(f)$	\check{r}_ℓ
5	5.3947(-7)	2.8464(-10)	5.3919(-7)
10	5.6156(-15)	3.9153(-19)	5.6152(-15)
20	2.8381(-33)	1.9697(-38)	2.8381(-33)
30	1.4386(-53)	2.3550(-59)	1.4386(-53)
40	3.1002(-76)	1.7644(-81)	3.1002(-76)
50	6.0499(-98)	1.4953(-104)	6.0499(-98)

magnitude of the quadrature errors

$$\tilde{\mathcal{E}}_\ell(f) = \mathcal{I}(f) - \tilde{\mathcal{G}}_\ell^{1,0}(f), \quad \check{\mathcal{E}}_{2\ell+1}(f) = \mathcal{I}(f) - \check{\mathcal{S}}_{2\ell+1}^{1,0}(f),$$

as well as the error estimates $\check{r}_\ell = \left| \check{\mathcal{S}}_{2\ell+1}^{1,0}(f) - \tilde{\mathcal{G}}_\ell^{1,0}(f) \right|$. Here $\check{\mathcal{S}}_{2\ell+1}^{1,0}$ stands for the optimal generalized averaged Gauss rule of Radau-type. The Radau-Kronrod rule $\mathcal{K}_{2\ell+1}^{1,0}(f)$ does not exist for the integrand and weight function of this example. The error estimates \check{r}_ℓ are very accurate. Moreover, the quadrature errors $\check{\mathcal{E}}_{2\ell+1}(f)$ are smaller than the errors $\tilde{\mathcal{E}}_\ell(f)$, as can be expected.

Example 5. This example is concerned with the integral

$$\mathcal{I}(f) = \int_{-1}^1 f(x) w_{-1/2,5}(x) dx, \quad f(x) = \frac{1}{1+25x^2}, \quad (72)$$

which differs from the integral (71) in the choice of weight function. Here $\mathcal{I}(f) \approx 2.4069503$. Table 7 shows the magnitude of the quadrature errors

$$\tilde{\mathcal{E}}_\ell(f) = \mathcal{I}(f) - \tilde{\mathcal{G}}_\ell^{1,1}(f), \quad \check{\mathcal{E}}_{2\ell+1}(f) = \mathcal{I}(f) - \check{\mathcal{S}}_{2\ell+1}^{1,1}(f),$$

where $\check{\mathcal{S}}_{2\ell+1}^{1,1}(f)$ denotes the optimal generalized averaged Gauss rule of Lobatto-type with fixed nodes at $x = \pm 1$. The table also displays the error estimates

$$\check{r}_\ell = \left| \check{\mathcal{S}}_{2\ell+1}^{1,1}(f) - \tilde{\mathcal{G}}_\ell^{1,1}(f) \right|,$$

which can be seen to be very accurate.

Example 6. Generalized averaged Gauss quadrature formulas may yield higher accuracy than Gauss quadrature rules that use the same moment information. This is illustrated in [20]. They therefore may be attractive

Table 7: Example 5: Results for the integral (72).

ℓ	$\tilde{\mathcal{E}}_\ell(f)$	$\check{\mathcal{E}}_{2\ell+1}(f)$	\check{r}_ℓ
5	4.7590(-2)	4.4396(-3)	4.3150(-2)
10	7.5213(-3)	1.6883(-5)	7.5044(-3)
20	1.0952(-4)	6.8036(-8)	1.0945(-4)
30	1.6694(-6)	2.0490(-10)	1.6692(-6)
40	2.7028(-8)	8.2724(-13)	2.7027(-8)
50	4.5494(-10)	2.7160(-15)	4.5494(-10)
60	7.8560(-12)	1.2226(-17)	7.8560(-12)

to use when moments or modified moments are cumbersome to evaluate. However, generalized averaged Gauss quadrature formulas may have nodes outside the convex hull of the support of the measure that defines the associated Gauss rules; see, e.g., [5, 6, 8] for examples and analyses. It may therefore not be possible to use generalized averaged Gauss quadrature formulas with integrands that only are defined on the convex hull of the support of the measure. This example illustrates this for the integral

$$\mathcal{I}(f) = \int_{-1}^1 f(x) w_{-0.8,3}(x) dx, \quad f(x) = 999.1^{\log_{10}(1-x)}. \quad (73)$$

The integrand f is defined only for $x < 1$, but we may use that $f(1) = \lim_{x \rightarrow 1^-} f(x) = 0$. We calculated the averaged Gauss rule and the optimal generalized averaged Gauss rule in the cases reported in Table 8, and we found that the largest node for these rules is larger than 1. These rules therefore cannot be applied. The internality of both these rules is analyzed in [16, 21] for Jacobi weight functions $w_{s,t}$ (68). We note that “the feasibility area”, i.e., the subset of the set $\{(s,t) \mid -1 < s, t < +\infty\} \subset \mathbb{R}$ in which the corresponding averaged Gauss rule is internal, displayed by the graphs in the cited papers, refers to the larger values of s and t . Since the “free” nodes of the generalized Gauss rule of Lobatto or Radau type $\check{\mathcal{S}}_{2\ell+1}^{p,q}$ associated with the weight function $w_{s,t}$ are the nodes of the corresponding generalized averaged Gauss rule $\check{\mathcal{S}}_{2\ell+1}$ associated with the Jacobi weight function $w_{s+p,t+q}(x) = (1-x)^{s+q}(1+x)^{t+p}$, we can make the rule $\check{\mathcal{S}}_{\ell+1}^{p,q}$ internal by increasing p or q . The quadrature rules $\check{\mathcal{S}}_{\ell+1}^{1,1}$ used to produce Table 8 are internal. Here they are the optimal generalized averaged Gauss rules of Lobatto type. The values of p and q used for the table are $p = 1$ and $q = 1$.

Table 8: Example 3.6: Results for the integral (73).

ℓ	$\tilde{\mathcal{E}}_\ell(f)$	$\check{\mathcal{E}}_{2\ell+1}(f)$	\check{r}_ℓ
5	4.2208(-8)	8.9891(-10)	4.3107(-8)
10	1.2119(-9)	1.2320(-11)	1.2242(-9)
20	2.5666(-11)	9.7843(-14)	2.5764(-11)
30	2.3969(-12)	4.9252(-15)	2.4018(-12)
40	4.2826(-13)	5.7260(-16)	4.2884(-13)

The free nodes of the rule $\check{\mathcal{S}}_{\ell+1}^{1,1}$ are in fact the nodes of the corresponding rule $\check{\mathcal{S}}_{2\ell+1}$ with respect to the Jacobi measure $w_{0.2,4}(x) = (1-x)^{0.2}(1+x)^4$.

Table 8 displays the magnitude of the quadrature errors

$$\tilde{\mathcal{E}}_\ell(f) = \mathcal{I}(f) - \tilde{\mathcal{G}}_\ell^{1,1}(f), \quad \check{\mathcal{E}}_{2\ell+1}(f) = \mathcal{I}(f) - \check{\mathcal{S}}_{2\ell+1}^{1,1}(f),$$

where $\check{\mathcal{S}}_{2\ell+1}^{1,1}$ is the optimal generalized averaged Gauss rule of Lobatto-type.

Moreover, the table shows error estimates $\check{r}_\ell = \left| \check{\mathcal{S}}_{2\ell+1}^{1,1}(f) - \tilde{\mathcal{G}}_\ell^{1,1}(f) \right|$, which are seen to be accurate. The quadrature rule $\mathcal{K}_{2\ell+1}^{1,1}(f)$ does not exist for the cases reported in Table 8. Here $\mathcal{I}(f) \approx 1.0180726$.

5. Conclusion

The optimal generalized averaged Gauss quadrature rules introduced in [21] are associated with Gauss quadrature rules. This paper describes extensions that are associated with Gauss-Radau and Gauss-Lobatto rules. Computed examples show these extensions to yield accurate estimates of the quadrature errors in Gauss-Radau and Gauss-Lobatto rules. The quadrature errors in Gauss-Radau and Gauss-Lobatto rules also may be estimated by using Radau-Kronrod or Lobatto-Kronrod described in [3, 17], however, the latter rules are more complicated to compute and, in fact, may not exist for certain weight functions.

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