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Rational averaged Gauss quadrature rules

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Dedicated to Academician Professor Gradimir Milovanović on the occasion of his 70th birthday.

Abstract. It is important to be able to estimate the quadrature error in Gauss rules. Several approaches have been developed, including the evaluation of associated Gauss-Kronrod rules (if they exist), or the associated averaged Gauss and generalized averaged Gauss rules. Integrals with certain integrands can be approximated more accurately by rational Gauss rules than by Gauss rules. This paper introduces associated rational averaged Gauss rules and rational generalized averaged Gauss rules, which can be used to estimate the error in rational Gauss rules. Also rational Gauss-Kronrod rules are discussed. Computed examples illustrate the accuracy of the error estimates determined by these quadrature rules.

1. Introduction

Let $\mathbb{P}_j$ denote the space of polynomials of degree at most j and let $d\lambda$ be a positive measure with $[a, b] = \mathrm{supp}(d\lambda)$. The n-point Gauss quadrature formula associated with $d\lambda$,

$$I(f) = \int_{\mathbb{R}} f(t)\, d\lambda(t) = G_n(f) + R_n^G(f), \quad G_n(f) = \sum_{\nu=1}^{n} \lambda_\nu^G f(\tau_\nu^G),$$

is the unique n-point quadrature rule with polynomial degree of exactness $2n-1$, i.e., the remainder satisfies

$$R_n^G(\mathbb{P}_{2n-1}) = 0.$$

Consider the monic orthogonal polynomials, $p_0, p_1, p_2, \ldots$, with respect to the inner product

$$(g, h) = \int_{\mathbb{R}} g(t)h(t)\, d\lambda(t).$$

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They satisfy a three-term recurrence relation

$$p_{i+1}(t) = (t - \alpha_i)p_i(t) - \beta_i p_{i-1}(t), \qquad i = 0, 1, 2, \dots ,$$

with $p_{-1}(t) \equiv 0$ and $p_0(t) \equiv 1$. The recursion coefficients α_i and $\beta_i > 0$ that define the polynomials p_n determine the symmetric tridiagonal Jacobi matrix

$$J_n = J_n(d\lambda) = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & 0 \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & \\ & \ddots & \ddots & \ddots & \\ & & \sqrt{\beta_{n-2}} & \alpha_{n-2} & \sqrt{\beta_{n-1}} \\ 0 & & & \sqrt{\beta_{n-1}} & \alpha_{n-1} \end{bmatrix}.$$

Golub and Welsch [12] developed an efficient algorithm for the computation of the nodes and weights of G_n. This algorithm is based on the observations that the nodes of G_n are the eigenvalues of the matrix J_n, and the weights are proportional to the squares of the first component of the corresponding normalized eigenvectors. The algorithm requires only $O(n^2)$ arithmetic floating points operations (flops) to compute the nodes and weights of G_n.

In practical applications of a Gauss rule G_n, it is important to be able to estimate the error $|(I - G_n)(f)|$. Many techniques for this purpose have been proposed in the literature; see, e.g., [9, 15–18]. The present paper focuses on error estimation methods that are determined by extensions of G_n, that inherit the n nodes of G_n. This property makes the computation of the error estimate economical. The best known extension of G_n of this kind is the $(2n + 1)$-point Gauss-Kronrod quadrature formula,

$$I(f) = \int_{\mathbb{R}} f(t)\,d\lambda(t) = K_n(f) + R_n^K(f), \quad K_n(f) = \sum_{\nu=1}^{n} \lambda_\nu^{GK} f(\tau_\nu^G) + \sum_{\mu=1}^{n+1} \lambda_\mu^K f(\tau_\mu^K).$$

Its polynomial degree of exactness is at least $3n + 1$, i.e.,

$$R_n^K(\mathbb{P}_{3n+1}) = 0.$$

The Gauss-Kronrod quadrature rule is commonly used to estimate the error in $G_n(f)$ by

$$|R_n^G(f)| = |(I - G_n)(f)| \approx |(K_n - G_n)(f)|. \tag{1}$$

The nodes $\{\tau_\nu^G\}_{\nu=1}^n$ of the Gauss-Kronrod rule are the nodes of G_n. We refer to the remaining nodes, $\{\tau_\mu^K\}_{\mu=1}^{k+1}$, as the Kronrod nodes. It is possible to compute the nodes and weights of Gauss-Kronrod rules efficiently by methods described in [1, 2, 14]. The method proposed by Laurie [14] uses the Golub-Welsch algorithm. A nice recent discussion on many properties of Gauss-Kronrod quadrature rules is provided by Notaris [18].

Ideally, the Kronrod nodes $\{\tau_\mu^K\}_{\mu=1}^{n+1}$ are real. This enhances their usefulness, because the use of complex-valued Kronrod nodes requires that the integrand can be defined in the complex plane by analytic continuation from the interval $[a, b]$. Unfortunately, there are several known situations when the Kronrod nodes are complex; see, e.g., [1, 18] for discussions and references. For this reason alternatives to Gauss-Kronrod quadrature rules for the estimation of the error in $G_n(f)$ have been developed. One of these is the $(2n + 1)$-point averaged Gauss quadrature formula introduced by Laurie [13],

$$I(f) = \int_{\mathbb{R}} f(t)\,d\lambda(t) = L_n(f) + R_n^L(f), \quad L_n(f) = \sum_{\nu=1}^{n} \lambda_\nu^{GL} f(\tau_\nu^G) + \sum_{\mu=1}^{n+1} \lambda_\mu^L f(\tau_\mu^L), \tag{2}$$

with polynomial degree of exactness at least $2n + 1$, i.e.,

$$R_n^L(\mathbb{P}_{2n+1}) = 0.$$

The symmetric tridiagonal Jacobi matrix associated with the quadrature rule (2) is given by (cf. [21])

$$J_n^L = J_n^L(d\lambda) = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & & & & & & & 0 \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & & & & & & & \\ & \ddots & \ddots & \ddots & & & & & & & \\ & & \sqrt{\beta_{n-1}} & \alpha_{n-1} & \sqrt{\beta_n} & & & & & & \\ & & & \sqrt{\beta_n} & \alpha_n & \sqrt{\beta_n} & & & & & \\ & & & & \sqrt{\beta_n} & \alpha_{n-1} & \sqrt{\beta_{n-1}} & & & & \\ & & & & & \sqrt{\beta_{n-1}} & \alpha_{n-2} & \sqrt{\beta_{n-2}} & & & \\ & & & & & & \ddots & \ddots & \ddots & & \\ & & & & & & & \sqrt{\beta_2} & \alpha_1 & \sqrt{\beta_1} \\ 0 & & & & & & & & \sqrt{\beta_1} & \alpha_0 \end{bmatrix}.$$

It follows that the nodes and weights of the rule (2) can be computed with the aid of the Golub-Welsch algorithm applied to the above matrix in $O(n^2)$ flops. The error of $G_n(f)$ can be estimated by

$$|R_n^G(f)| = |(I - G_n)(f)| \approx |(L_n - G_n)(f)|. \tag{3}$$

Spalević [21], by using results on the characterization of positive quadrature rules by Peherstorfer [20], proposed a modification of the quadrature rule (2),

$$I(f) = \int_{\mathbb{R}} f(t)\, d\lambda(t) = S_n(f) + R_n^S(f), \quad S_n(f) = \sum_{\nu=1}^{n} \lambda_\nu^{GS} f(\tau_\nu^G) + \sum_{\mu=1}^{n+1} \lambda_\mu^S f(\tau_\mu^S), \tag{4}$$

which he referred to as a generalized averaged Gauss quadrature formula. It has polynomial degree of exactness at least $2n + 2$, i.e.,

$$R_n^S(\mathbb{P}_{2n+2}) = 0.$$

When the measure $d\lambda$ is even on its support $[-c, c]$ ($c > 0$), S_n has polynomial degree of exactness at least $2n + 3$. The symmetric tridiagonal Jacobi matrix associated with the quadrature rule (4) takes the form

$$J_n^S = J_n^S(d\lambda) = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & & & & & & & 0 \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & & & & & & & \\ & \ddots & \ddots & \ddots & & & & & & & \\ & & \sqrt{\beta_{n-1}} & \alpha_{n-1} & \sqrt{\beta_n} & & & & & & \\ & & & \sqrt{\beta_n} & \alpha_n & \sqrt{\beta_{n+1}} & & & & & \\ & & & & \sqrt{\beta_{n+1}} & \alpha_{n-1} & \sqrt{\beta_{n-1}} & & & & \\ & & & & & \sqrt{\beta_{n-1}} & \alpha_{n-2} & \sqrt{\beta_{n-2}} & & & \\ & & & & & & \ddots & \ddots & \ddots & & \\ & & & & & & & \sqrt{\beta_2} & \alpha_1 & \sqrt{\beta_1} \\ 0 & & & & & & & & \sqrt{\beta_1} & \alpha_0 \end{bmatrix}.$$

Hence, the nodes and weights of the rule (4) also can be computed efficiently with the Golub-Welsch algorithm in $O(n^2)$ flops. The rule (4) also can be used to estimate the error in $G_n(f)$. We have the error estimate

$$|R_n^G(f)| = |(I - G_n)(f)| \approx |(S_n - G_n)(f)|. \tag{5}$$

When the measure $d\lambda$ is positive, both L_n and S_n have lower polynomial degree of exactness than K_n, but L_n and S_n always exist with real nodes $\{\tau_\mu^L\}_{\mu=1}^{n+1}$ and $\{\tau_\mu^S\}_{\mu=1}^{n+1}$, respectively, that alternate with the Gauss nodes $\{\tau_\nu^G\}_{\nu=1}^n$. Besides, all weights of the rules L_n and S_n are positive. Moreover, the rules L_n and S_n are easier to compute than the rule K_n when the latter exists. Further results on quadrature rules based on the construction from [21] and their relation to Gauss-Kronrod quadrature rules can be found in [3–5, 19, 22–24].

The Gauss formula G_n and its extensions K_n, L_n, and S_n give high accuracy when the integrand can be approximated well by a polynomial of small to moderate degree. However, this is not the case when the integrand has poles or other singularities close to the support of the measure $d\lambda$. In this situation, it is natural to require that the quadrature rule is exact not only for all polynomials of a certain degree, but also for elementary rational functions with poles close to or at the singularities of the integrand. It is the purpose of the present paper to develop analogues of the quadrature rules (2) and (4) with this property.

This paper is organized as follows. Section 2 recalls some known results on rational Gauss-type quadrature rules. In Section 3, we introduce rational averaged Gauss quadrature formulas and rational generalized averaged Gauss quadrature formulas. Section 4 discusses the application of these rules to the estimation of the error in rational Gauss quadrature rules, and presents computed examples. Concluding remarks can be found in Section 5.

2. Rational Gauss-type quadrature formulas

Let $\{\zeta_\mu\}_{\mu=1}^M$ be a set of distinct nonvanishing real or complex numbers such that

$$1 + \zeta_\mu t \neq 0 \quad \text{for} \quad t \in [a, b], \quad \mu = 1, 2, \ldots, M. \tag{6}$$

Typically, the ζ_μ are real or appear in complex conjugate pairs. Let d be a nonnegative integer, and let m be an integer such that $0 \leq m \leq d$. Introduce the m-dimensional linear space of rational functions

$$\mathbb{Q}_m = \operatorname{span}\left\{ r : \ r(t) = \frac{1}{(1+\zeta_\mu t)^s}, \ s = 1, 2, \ldots, s_\mu, \ \mu = 1, 2, \ldots, M, \ \sum_{\mu=1}^M s_\mu = m \right\}$$

and define the linear space

$$\mathbb{S}_d = \mathbb{Q}_m \oplus \mathbb{P}_{d-1-m} \tag{7}$$

of dimension d. We are interested in N-point quadrature rules

$$I(f) = \int_{\mathbb{R}} f(t)\, d\lambda(t) = Q_{N,m}(f) + R_{N,m}(f), \quad Q_{N,m}(f) = \sum_{\nu=1}^N \widetilde{\lambda}_\nu f(\widetilde{\tau}_\nu), \tag{8}$$

that are exact for all functions in the linear space (7). The following result is stated by Gautschi [8]:

Theorem 2.1. *Assume that the distinct points* $\{\zeta_\mu\}_{\mu=1}^M$ *satisfy* (6)*, and let* $0 \leq m \leq d$*. Define the polynomial, of exact degree* m*,*

$$\omega_m(t) = \prod_{\mu=1}^M (1 + \zeta_\mu t)^{s_\mu}$$

and the modified measure

$$d\widetilde{\lambda} = \frac{d\lambda}{\omega_m}.$$

Assume that this measure admits an N*-point quadrature formula of polynomial degree of exactness* $d-1$*,*

$$\int_{\mathbb{R}} p(t)\, d\widetilde{\lambda}(t) = \sum_{\nu=1}^N \lambda_\nu f(\tau_\nu) \quad \text{for all} \quad p \in \mathbb{P}_{d-1}, \tag{9}$$

Define

$$\widetilde{\tau}_\nu = \tau_\nu, \quad \widetilde{\lambda}_\nu = \lambda_\nu \omega_m(\tau_\nu), \quad \nu = 1, 2, \ldots, N, \tag{10}$$

Then the quadrature formula (8) *satisfies*

$$R_{N,m}(\mathbb{S}_d) = 0 \tag{11}$$

with $\mathbb{S}_d$ *defined by* (7).

Conversely, if (8) *and* (11) *hold with pairwise distinct nodes* $\widetilde{\tau}_\nu \in [a, b]$, *then so does* (9) *with* τ_ν *and* λ_ν *given by* (10).

For $N = n$ and $d = 2n$, we have $0 \leq m \leq 2n$ and $\mathbb{S}_{2n} = \mathbb{Q}_m \oplus \mathbb{P}_{2n-1-m}$. This special case of Theorem 2.1 is shown by Gautschi [9, Theorem 3.25]; see also [6]. It leads the construction of the n-point rational Gauss quadrature formula

$$I(f) = \int_{\mathbb{R}} f(t)\, d\lambda(t) = G_{n,m}(f) + R^G_{n,m}(f), \quad G_{n,m}(f) = \sum_{\nu=1}^{n} \widetilde{\lambda}^G_\nu f(\widetilde{\tau}^G_\nu), \quad R^G_{n,m}(\mathbb{S}_{2n}) = 0.$$

The nodes and weights of $G_{n,m}$ are obtained as

$$\widetilde{\tau}^G_\nu = \tau^{\widetilde{G}}_\nu, \quad \widetilde{\lambda}^G_\nu = \lambda^{\widetilde{G}}_\nu \omega_m(\tau^{\widetilde{G}}_\nu), \quad \nu = 1, 2, \ldots, n,$$

where $\tau^{\widetilde{G}}_\nu$ and $\lambda^{\widetilde{G}}_\nu$ are the nodes and weights of the n-point (polynomial) Gauss quadrature formula associated with the measure $d\widetilde{\lambda} = d\lambda/\omega_m$.

The situation when $N = 2n+1$ and $d = 3n+2$, with $0 \leq m \leq 3n+2$, is discussed by Gautschi [9, Theorem 3.41] and in [11]. In this case, $\mathbb{S}_{3n+2} = \mathbb{Q}_m \oplus \mathbb{P}_{3n+1-m}$, which leads to the construction of the $(2n+1)$-point rational Gauss-Kronrod quadrature formula. Thus, let $N = 2n+1$ and $d = 3n+2$. We then obtain the $(2n+1)$-point rational Gauss-Kronrod quadrature formula

$$I(f) = \int_{\mathbb{R}} f(t)\, d\lambda(t) = K_{n,m}(f) + R^K_{n,m}(f), \quad K_{n,m}(f) = \sum_{\nu=1}^{n} \widetilde{\lambda}^{GK}_\nu f(\widetilde{\tau}^G_\nu) + \sum_{\mu=1}^{n+1} \widetilde{\lambda}^K_\mu f(\widetilde{\tau}^K_\mu), \quad R^K_{n,m}(\mathbb{S}_{3n+2}) = 0.$$

Its nodes and weights are given by

$$\widetilde{\tau}^G_\nu = \tau^{\widetilde{G}}_\nu, \quad \widetilde{\tau}^K_\mu = \tau^{\widetilde{K}}_\mu, \qquad \widetilde{\lambda}^{GK}_\nu = \lambda^{\widetilde{GK}}_\nu \omega_m(\tau^{\widetilde{G}}_\nu), \quad \widetilde{\lambda}^K_\mu = \lambda^{\widetilde{K}}_\mu \omega_m(\tau^{\widetilde{K}}_\mu), \qquad \nu = 1, 2, \ldots, n, \quad \mu = 1, 2, \ldots, n+1,$$

where $\tau^{\widetilde{G}}_\nu$ and $\tau^{\widetilde{K}}_\mu$ are the nodes, while $\lambda^{\widetilde{GK}}_\nu$ and $\lambda^{\widetilde{K}}_\mu$ are the weights, of $(2n+1)$-point (polynomial) Gauss-Kronrod quadrature formula associated with the measure $d\widetilde{\lambda} = d\lambda/\omega_m$.

Theorem 2.1 can be shown for other choices of d and N in a similar manner as the proof of Gautschi [9, Theorem 3.25].

3. Rational averaged and generalized averaged Gauss quadrature formulas

Let $\widetilde{\alpha}_i$, $i = 0, 1, 2, \ldots$, and $\widetilde{\beta}_i$, $i = 1, 2, 3, \ldots$, be the coefficients of the three-term recurrence relation satisfied by the monic orthogonal polynomials with respect to the measure $d\widetilde{\lambda}$. The nodes of the n-point Gauss rule associated with this measure are the eigenvalues of the symmetric tridiagonal Jacobi matrix

$$J_n(d\widetilde{\lambda}) = \begin{bmatrix} \widetilde{\alpha}_0 & \sqrt{\widetilde{\beta}_1} & & & 0 \\ \sqrt{\widetilde{\beta}_1} & \widetilde{\alpha}_1 & \sqrt{\widetilde{\beta}_2} & & \\ & \ddots & \ddots & \ddots & \\ & & \sqrt{\widetilde{\beta}_{n-2}} & \widetilde{\alpha}_{n-2} & \sqrt{\widetilde{\beta}_{n-1}} \\ 0 & & & \sqrt{\widetilde{\beta}_{n-1}} & \widetilde{\alpha}_{n-1} \end{bmatrix};$$

cf. the discussion in Section 1.

Consider the special case of Theorem 2.1 when $N = 2n+1$ and $d = 2n+2$, with $0 \le m \le 2n+2$ and $\mathbb{S}_{2n+2} = \mathbb{Q}_m \oplus \mathbb{P}_{2n+1-m}$. We obtain the $(2n+1)$-point rational averaged Gauss quadrature formula

$$I(f) = \int_{\mathbb{R}} f(t)\, d\lambda(t) = L_{n,m}(f) + R^L_{n,m}(f), \quad L_{n,m}(f) = \sum_{\nu=1}^{n} \widetilde{\lambda}_\nu^{GL} f(\widetilde{\tau}_\nu^G) + \sum_{\mu=1}^{n+1} \widetilde{\lambda}_\mu^{L} f(\widetilde{\tau}_\mu^L), \quad R^L_{n,m}(\mathbb{S}_{2n+2}) = 0.$$

The nodes and the weights of $L_{n,m}$ are obtained as

$$\widetilde{\tau}_\nu^G = \tau_\nu^{\widetilde{G}}, \quad \widetilde{\tau}_\mu^L = \tau_\mu^{\widetilde{L}}, \qquad \widetilde{\lambda}_\nu^{GL} = \lambda_\nu^{\widetilde{GL}} \omega_m(\tau_\nu^{\widetilde{G}}), \quad \widetilde{\lambda}_\mu^{L} = \lambda_\mu^{\widetilde{L}} \omega_m(\tau_\mu^{\widetilde{L}}), \qquad \nu = 1,2,\ldots,n, \quad \mu = 1,2,\ldots,n+1,$$

where $\tau_\nu^{\widetilde{G}}$ and $\tau_\mu^{\widetilde{L}}$ are the nodes, while $\lambda_\nu^{\widetilde{GL}}$ and $\lambda_\mu^{\widetilde{L}}$ are the weights, of the $(2n+1)$-point (polynomial) averaged Gauss quadrature formula associated with the measure $d\widetilde{\lambda} = d\lambda/\omega_m$. The nodes are the eigenvalues and the weights are proportional to the squares of the first component of associated normalized eigenvectors of the matrix

$$J_n^L(d\widetilde{\lambda}) = \begin{bmatrix} \widetilde{\alpha}_0 & \sqrt{\widetilde{\beta}_1} & & & & & & & & & 0 \\ \sqrt{\widetilde{\beta}_1} & \widetilde{\alpha}_1 & \sqrt{\widetilde{\beta}_2} & & & & & & & & \\ & \ddots & \ddots & \ddots & & & & & & & \\ & & \sqrt{\widetilde{\beta}_{n-1}} & \widetilde{\alpha}_{n-1} & \sqrt{\widetilde{\beta}_n} & & & & & & \\ & & & \sqrt{\widetilde{\beta}_n} & \widetilde{\alpha}_n & \sqrt{\widetilde{\beta}_n} & & & & & \\ & & & & \sqrt{\widetilde{\beta}_n} & \widetilde{\alpha}_{n-1} & \sqrt{\widetilde{\beta}_{n-1}} & & & & \\ & & & & & \sqrt{\widetilde{\beta}_{n-1}} & \widetilde{\alpha}_{n-2} & \sqrt{\widetilde{\beta}_{n-2}} & & & \\ & & & & & & \ddots & \ddots & \ddots & & \\ & & & & & & & \sqrt{\widetilde{\beta}_2} & \widetilde{\alpha}_1 & \sqrt{\widetilde{\beta}_1} & \\ 0 & & & & & & & & \sqrt{\widetilde{\beta}_1} & \widetilde{\alpha}_0 & \end{bmatrix}.$$

It follows that the nodes and the weights can be computed in only $O(n^2)$ flops by the Golub-Welsch algorithm.

The special case of Theorem 2.1 when $N = 2n+1$ and $d = 2n+3$, with $0 \le m \le 2n+3$ and $\mathbb{S}_{2n+3} = \mathbb{Q}_m \oplus \mathbb{P}_{2n+2-m}$, gives the $(2n+1)$-point rational generalized averaged Gauss quadrature formula

$$I(f) = \int_{\mathbb{R}} f(t)\, d\lambda(t) = S_{n,m}(f) + R^S_{n,m}(f), \quad S_{n,m}(f) = \sum_{\nu=1}^{n} \widetilde{\lambda}_\nu^{GS} f(\widetilde{\tau}_\nu^G) + \sum_{\mu=1}^{n+1} \widetilde{\lambda}_\mu^{S} f(\widetilde{\tau}_\mu^S), \quad R^S_{n,m}(\mathbb{S}_{2n+3}) = 0.$$

When the weight function is even, we may choose $d = 2n+4$, so $0 \le m \le 2n+4$ and $\mathbb{S}_{2n+4} = \mathbb{Q}_m \oplus \mathbb{P}_{2n+3-m}$. Then we have $R^S_{n,m}(\mathbb{S}_{2n+4}) = 0$. The nodes and weights of $S_{n,m}$ are given by

$$\widetilde{\tau}_\nu^G = \tau_\nu^{\widetilde{G}}, \quad \widetilde{\tau}_\mu^S = \tau_\mu^{\widetilde{S}}, \qquad \widetilde{\lambda}_\nu^{GS} = \lambda_\nu^{\widetilde{GS}} \omega_m(\tau_\nu^{\widetilde{G}}), \quad \widetilde{\lambda}_\mu^{S} = \lambda_\mu^{\widetilde{S}} \omega_m(\tau_\mu^{\widetilde{S}}), \qquad \nu = 1,2,\ldots,n, \quad \mu = 1,2,\ldots,n+1,$$

where $\tau_\nu^{\widetilde{G}}$ and $\tau_\mu^{\widetilde{S}}$ are the nodes, and $\lambda_\nu^{\widetilde{GS}}$ and $\lambda_\mu^{\widetilde{S}}$ are the weights, of the $(2n+1)$-point (polynomial) generalized averaged Gauss quadrature formula associated with the measure $d\widetilde{\lambda} = d\lambda/\omega_m$. The nodes and weights can be computed by applying the Golub-Welsch algorithm to the matrix

$$J_n^S(d\widetilde{\lambda}) = \begin{bmatrix} \widetilde{\alpha}_0 & \sqrt{\widetilde{\beta}_1} & & & & & & & & & 0 \\ \sqrt{\widetilde{\beta}_1} & \widetilde{\alpha}_1 & \sqrt{\widetilde{\beta}_2} & & & & & & & & \\ & \ddots & \ddots & \ddots & & & & & & & \\ & & \sqrt{\widetilde{\beta}_{n-1}} & \widetilde{\alpha}_{n-1} & \sqrt{\widetilde{\beta}_n} & & & & & & \\ & & & \sqrt{\widetilde{\beta}_n} & \widetilde{\alpha}_n & \sqrt{\widetilde{\beta}_{n+1}} & & & & & \\ & & & & \sqrt{\widetilde{\beta}_{n+1}} & \widetilde{\alpha}_{n-1} & \sqrt{\widetilde{\beta}_{n-1}} & & & & \\ & & & & & \sqrt{\widetilde{\beta}_{n-1}} & \widetilde{\alpha}_{n-2} & \sqrt{\widetilde{\beta}_{n-2}} & & & \\ & & & & & & \ddots & \ddots & \ddots & & \\ & & & & & & & \sqrt{\widetilde{\beta}_2} & \widetilde{\alpha}_1 & \sqrt{\widetilde{\beta}_1} & \\ 0 & & & & & & & & \sqrt{\widetilde{\beta}_1} & \widetilde{\alpha}_0 & \end{bmatrix}.$$

We note that the polynomial quadrature formulas G_n, K_n, L_n, and S_n are special cases of the rational quadrature formulas $G_{n,m}$, $K_{n,m}$, $L_{n,m}$, and $S_{n,m}$, respectively, for $m = 0$.

It follows from Theorem 2.1 that the construction of rational quadrature formulas for the measure $d\lambda$ comes down to the construction of the corresponding polynomial quadrature rules for the modified measure $d\widetilde{\lambda} = d\lambda/\omega_m$. If this polynomial quadrature rule is not internal (i.e., if one or several of its nodes are outside the interval $[a, b]$), then, if a pole coincides with a node, our construction of the desired rational quadrature rule may have to be modified. This difficulty easily can be remedied by moving the problematic pole.

We remark that the modified measure $d\widetilde{\lambda}$ does not have to be real-valued and of constant sign on $[a, b]$ (in fact, it may be complex-valued, since the poles ζ_μ may be complex). However, Gauss quadrature rules associated with a complex-valued measure are not guaranteed to exist. When all poles are real and outside the interval $[a, b]$, or appear in complex conjugate pairs, the measure $d\widetilde{\lambda}$ is of constant sign on $[a, b]$ and the required quadrature rules exist.

We turn to the existence and internality of quadrature rules considered. Assume that the measure $d\widetilde{\lambda}$ is real-valued and of constant sign on the interval $[a, b]$. It is well known that the polynomial Gauss-Kronrod quadrature formula might neither be internal nor have real nodes; see [18] for a recent discussion and references. This also holds for rational Gauss-Kronrod quadrature rules. The averaged and generalized averaged polynomial quadrature rules always exist, but might not be internal. This issue is investigated and illustrated for several special measures in [3–5, 21].

4. Error estimates for rational Gauss quadrature formulas

We mentioned in Section 1 that the polynomial quadrature rules K_n, L_n, and S_n may be used to estimate the error in the Gauss rule G_n; see (1), (3), and (5). All these error estimations are economical in the sense that the quadrature rules K_n, L_n, and S_n inherit the n nodes of G_n.

In this paper we are interested in applying the rational quadrature rule $K_{n,m}$, $L_{n,m}$, and $S_{n,m}$ to estimate the error in the rational Gauss rule $G_{n,m}$. If the measure $d\widetilde{\lambda}$ defined in Theorem 2.1 is used for the construction of $G_{n,m}$, as well as of $K_{n,m}$, $L_{n,m}$, and $S_{n,m}$, then this secures that the rules $K_{n,m}$, $L_{n,m}$, and $S_{n,m}$ inherit n nodes ($\widetilde{\tau}_\nu^G$) from $G_{n,m}$ making the error estimates economical. This can be accomplished by using the the same integer m and the same space $\mathbb{Q}_m$ for all four kinds of rational quadrature rules considered. This means that the quadrature rules $K_{n,m}$, $L_{n,m}$, and $S_{n,m}$ will have the same rational degree, but higher polynomial degree, of exactness, as $G_{n,m}$. The permitted values of m are $0 \le m \le 2n$.

We write the formulas for error estimation in the form

$$|R^G_{n,m}(f)| = |(I - G_{n,m})(f)| \approx |(K_{n,m} - G_{n,m})(f)|,$$

$$|R^G_{n,m}(f)| = |(I - G_{n,m})(f)| \approx |(L_{n,m} - G_{n,m})(f)|,$$

$$|R^G_{n,m}(f)| = |(I - G_{n,m})(f)| \approx |(S_{n,m} - G_{n,m})(f)|.$$

The following numerical examples, in which the OPQ suite [10] is used, illustrate the performance of these estimates. The computations were carried out in MATLAB with about 15 significant decimal digits.

Example 1. In this example we consider the analytically computable integral

$$I = \int_{-1}^{1} \frac{dt}{\sqrt{2.2 - 0.9t - t^2}} = \arcsin\frac{29}{31} + \arcsin\frac{11}{31} \approx 1.572367443645470.$$

The integrand has two real simple poles defined by

$$-1/\zeta_1 = 1.1, \quad -1/\zeta_2 = -2.$$

We calculate the quadrature formulas $G_{n,m}$, $K_{n,m}$, $L_{n,m}$, and $S_{n,m}$ (which exist in all considered cases), compare them to the exact value of I by calculating the differences $|I - G_{n,m}|$, $|I - K_{n,m}|$, $|I - L_{n,m}|$, and $|I - S_{n,m}|$, and estimate the error of $G_{n,m}$ by the the differences $|K_{n,m} - G_{n,m}|$, $|L_{n,m} - G_{n,m}|$, and $|S_{n,m} - G_{n,m}|$, for $m = 0, 1, 2$ and $n = 2, 5, 7, 10$. In the case of $m = 1$ both $-1/\zeta_1 = 1.1$ and $-1/\zeta_2 = -2$ are considered. The results are shown in Table 1. This table shows the errors $|I - G_{n,m}|$, $|I - K_{n,m}|$, $|I - L_{n,m}|$, and $|I - S_{n,m}|$ to decrease for a fixed m as n is increased. A comparison of these differences shows that $K_{n,m}$ gives higher accuracy than $S_{n,m}$ and $S_{n,m}$, yields higher accuracy than $L_{n,m}$, and $L_{n,m}$ is more accurate than $G_{n,m}$ (except in some cases when $n = 2$). Comparing the error estimates $|K_{n,m} - G_{n,m}|$, $|L_{n,m} - G_{n,m}|$, and $|S_{n,m} - G_{n,m}|$ to the actual error $|I - G_{n,m}|$, we see that all the rules $K_{n,m}$, $L_{n,m}$, and $S_{n,m}$ give good estimates of the error in $G_{n,m}$.

The errors $|I - G_{n,m}|$, $|I - K_{n,m}|$, $|I - L_{n,m}|$, and $|I - S_{n,m}|$ generally are smaller when $m = 1$ and $-1/\zeta_1 = 1.1$ than when $m = 1$ and $-1/\zeta_2 = -2$. It can be difficult to predict how incorporating poles in quadrature rules will affect the accuracy of the rules. The error estimates $|K_{n,m} - G_{n,m}|$, $|L_{n,m} - G_{n,m}|$, and $|S_{n,m} - G_{n,m}|$ can help us to decide which poles to include to make the rational Gauss quadrature formula $G_{n,m}$ as accurate as possible.

Example 2. Consider the integral

$$\begin{aligned} I &= \int_{-1}^{1} \frac{\cos\frac{t}{2}}{\cos^5 t} dt \\ &= -4\left(\frac{35}{2^{17/2}} \ln\left|\frac{4\sin\frac{1}{2} - 2^{3/2}}{4\sin\frac{1}{2} + 2^{3/2}}\right| + \frac{840\sin^7\frac{1}{2} - 1540\sin^5\frac{1}{2} + 1022\sin^3\frac{1}{2} - 279\sin\frac{1}{2}}{6144\sin^8\frac{1}{2} - 12288\sin^6\frac{1}{2} + 9216\sin^4\frac{1}{2} - 3072\sin^2\frac{1}{2} + 384}\right) \\ &\approx 7.392300895896495. \end{aligned}$$

All poles of the integrand are real and of multiplicity 5. They can be written in the form

$$-\frac{1}{\zeta_\mu} = \pm(2l - 1)\frac{\pi}{2}, \quad l \in \mathbb{N}. \tag{12}$$

It is natural to let m be even and use the poles closest to and on both sides of the interval of integration. We carry out the same computations as in the previous example for $n = 3$ and $m = 0, 2, \ldots, 12$. For $m = 2, 4, 6, 8, 10$, we choose poles that in (12) correspond to $l = 1$ of multiplicity $1, 2, 3, 4, 5$, respectively, and for $m = 12$ we choose poles that correspond to $l = 1$ of multiplicity 5 and poles that correspond to $l = 2$ of multiplicity 1. Table 2 displays the computed results. Since $n = 3$, we do not have a theoretical justification for $m > 6$ in $G_{n,m}$, for $m > 8$ in $L_{n,m}$, for $m > 10$ in $S_{n,m}$ (since the weight function is even), and for $m > 11$ in $K_{n,m}$. However, the accuracy in all quadrature formulas increases with m (except that $K_{3,10}$ is more accurate than $K_{3,12}$). We observe that all the considered error estimates give good results.

$I = \int_{-1}^{1} \frac{dt}{\sqrt{2.2 - 0.9t - t^2}} \approx 1.572367443645470$								
m	n	$\lvert I - G_{n,m}\rvert$	$\lvert I - K_{n,m}\rvert$	$\lvert K_{n,m} - G_{n,m}\rvert$	$\lvert I - L_{n,m}\rvert$	$\lvert L_{n,m} - G_{n,m}\rvert$	$\lvert I - S_{n,m}\rvert$	$\lvert S_{n,m} - G_{n,m}\rvert$
0	2	6.3413e-02	5.6604e-04	6.2847e-02	7.1534e-04	6.4128e-02	5.6604e-04	6.2847e-02
0	5	3.0105e-03	7.3209e-06	3.0178e-03	2.6543e-05	3.0370e-03	2.0574e-05	3.0310e-03
0	7	4.4253e-04	3.9039e-07	4.4292e-04	1.6962e-06	4.4422e-04	1.3519e-06	4.4388e-04
0	10	2.6344e-05	3.8811e-09	2.6348e-05	3.4368e-08	2.6378e-05	2.6851e-08	2.6371e-05
1 (ζ_1)	2	1.0121e-02	6.9811e-04	1.0819e-02	1.9587e-04	1.0316e-02	8.3380e-05	1.0204e-02
1 (ζ_1)	5	2.7045e-04	1.1664e-07	2.7057e-04	6.0590e-07	2.7106e-04	2.9539e-07	2.7075e-04
1 (ζ_1)	7	2.7952e-05	2.8215e-09	2.7955e-05	3.3258e-08	2.7985e-05	1.8884e-08	2.7971e-05
1 (ζ_1)	10	1.1490e-06	4.1750e-11	1.1490e-06	6.5060e-10	1.1497e-06	4.0900e-10	1.1494e-06
1 (ζ_2)	2	7.8692e-02	2.2289e-03	7.6463e-02	2.8247e-04	7.8975e-02	1.1817e-03	7.7511e-02
1 (ζ_2)	5	3.7134e-03	9.9552e-06	3.7233e-03	3.5262e-05	3.7486e-03	2.8128e-05	3.7415e-03
1 (ζ_2)	7	5.4311e-04	5.4814e-07	5.4366e-04	2.2511e-06	5.4536e-04	1.8391e-06	5.4495e-04
1 (ζ_2)	10	3.2200e-05	5.2638e-09	3.2205e-05	4.4628e-08	3.2245e-05	3.5616e-08	3.2236e-05
2	2	2.3121e-02	1.0007e-03	2.4121e-02	3.3774e-04	2.3458e-02	4.6347e-04	2.3584e-02
2	5	3.5248e-04	3.2027e-07	3.5280e-04	8.0691e-07	3.5329e-04	4.7279e-07	3.5295e-04
2	7	3.5516e-05	6.2912e-09	3.5522e-05	4.3594e-08	3.5559e-05	2.7084e-08	3.5543e-05
2	10	1.4377e-06	5.0342e-11	1.4377e-06	8.4003e-10	1.4385e-06	5.5415e-10	1.4382e-06

Table 1: Calculations for Example 1.

$I = \int_{-1}^{1} \frac{\cos \frac{t}{2}}{\cos^5 t} dt \approx 7.392300895896495$								
n	m	$\lvert I - G_{n,m}\rvert$	$\lvert I - K_{n,m}\rvert$	$\lvert K_{n,m} - G_{n,m}\rvert$	$\lvert I - L_{n,m}\rvert$	$\lvert L_{n,m} - G_{n,m}\rvert$	$\lvert I - S_{n,m}\rvert$	$\lvert S_{n,m} - G_{n,m}\rvert$
3	0	9.8634e-01	2.9631e-03	9.8931e-01	1.2172e-02	9.9852e-01	7.3152e-03	9.9366e-01
3	2	6.3463e-01	2.5868e-03	6.3722e-01	4.7847e-03	6.3941e-01	3.1325e-03	6.3776e-01
3	4	3.5847e-01	1.4045e-03	3.5988e-01	1.3587e-03	3.5983e-01	5.8543e-04	3.5906e-01
3	6	1.6524e-01	5.0823e-04	1.6575e-01	3.7834e-04	1.6562e-01	1.8873e-04	1.6505e-01
3	8	5.0900e-02	9.9526e-05	5.1000e-02	1.5534e-04	5.1056e-02	1.2948e-04	5.0771e-02
3	10	1.3325e-03	5.0332e-09	1.3325e-03	1.8294e-06	1.3343e-03	8.4632e-08	1.3324e-03
3	12	7.9586e-04	7.9342e-09	7.9585e-04	8.2065e-07	7.9668e-04	1.4048e-08	7.9587e-04

Table 2: Calculations for Example 2.

$I = \int_0^\infty \frac{t^k \sqrt{1+\theta t/2}}{e^{-\eta} - e^{-t}} t^{k-1} e^{-t} dt, \quad \eta = -1, \ \theta = 1, \ k = 5/2$					
m	n	$G_{n,m}$	$\lvert K_{n,m} - G_{n,m}\rvert$	$\lvert L_{n,m} - G_{n,m}\rvert$	$\lvert S_{n,m} - G_{n,m}\rvert$
0	2	2.063020079887507	-	2.8922e-03	5.2860e-03
0	5	2.059594730987161	-	2.5304e-04	3.3970e-04
0	7	2.059377785222887	-	5.6105e-05	7.3338e-05
0	10	2.059325354240259	-	7.9601e-06	1.0082e-05
1	2	2.068253915837720	-	8.8504e-03	8.7643e-03
1	5	2.059302045808841	-	1.5005e-05	1.3904e-05
1	7	2.059317845147125	-	1.0231e-06	1.0201e-06
1	10	2.059316768475453	-	1.6087e-08	-
3	2	1.998440028870835	-	6.1002e-02	6.0882e-02
3	5	2.059315914991958	-	8.8412e-07	9.1595e-07
3	7	2.059316779964540	-	2.6303e-08	3.0938e-08
3	10	2.059316806712986	-	1.0604e-09	-
5	5	2.059316318353998	-	4.7331e-07	5.1435e-07
5	7	2.059316785983647	-	2.0914e-08	2.3833e-08
5	10	2.059316807138894	-	7.7277e-10	-
7	5	2.059316638891903	-	1.5524e-07	1.8982e-07
7	7	2.059316789669078	-	1.7445e-08	1.9732e-08
7	10	2.059316807330022	-	5.9073e-10	6.6784e-10

Table 3: Calculations for Example 3.

Example 3. We consider the generalized Bose-Einstein integral, which finds applications in solid state physics. Details on the computation of this integral are described by Gautschi [7, 9]. The generalized Bose-Einstein integral can be written in the form

$$I = \int_0^\infty \frac{t^k \sqrt{1+\theta t/2}}{e^{-\eta} - e^{-t}} t^{k-1} e^{-t} dt,$$

with three parameters $\eta < 0$, $\theta \geq 0$, and $k \in \left\{\frac{1}{2}, \frac{3}{2}, \frac{5}{2}\right\}$. For the measure of integration, we take the generalized Laguerre measure $d\lambda(t) = t^{k-1}e^{-t}dt$ on $[0, \infty)$. The integrand has infinitely many simple complex conjugate poles and one simple real pole. The poles are

$$\zeta_\mu = -\frac{1}{\eta + (\mu+1)i\pi}, \quad \zeta_{\mu+1} = -\frac{1}{\eta - (\mu+1)i\pi}, \quad \mu = 1, 3, \ldots, m-2, \quad \zeta_m = -\frac{1}{\eta}.$$

This suggests to let m be odd in the rational quadrature rules. An analytical expression for the Bose-Einstein integral is not known, but it can be approximated by $G_{n,m}$ if this quadrature rule exists. Selected results for $\eta = -1$, $\theta = 1$, $k = 5/2$, and different choices of n and m are displayed in Table 3. The Gauss-Kronrod rules $K_{n,m}$ do not exist in any of the considered cases, the rule $L_{n,m}$ exists in all considered cases, while $S_{n,m}$ exists in all considered cases except for $n = 10$ and $m = 1, 3, 5$. Table 3 shows $G_{n,m}$ and the error estimates $|L_{n,m} - G_{n,m}|$ and $|S_{n,m} - G_{n,m}|$ when they exist.

5. Conclusion

Rational Gauss-type quadrature formulas $K_{n,m}$, $L_{n,m}$, and $S_{n,m}$ can be used to estimate the error in the rational Gauss quadrature formula $G_{n,m}$ in an efficient manner. Rational Gauss-Kronrod rules have been introduced by Gautschi, Gori, and Lo Cascio [11]. The present paper introduces rational averaged and rational generalized averaged quadrature rules that may exist when rational Gauss-Kronrod rules do not. Numerical experiments confirm efficiency of the new error estimation techniques proposed.

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