



Rational Averaged Gauss Quadrature Rules

Lothar Reichel^a, Miodrag M. Spalević^b, Jelena D. Tomanović^{b,*}

^aDepartment of Mathematical Sciences, Kent State University, Kent, OH 44242, USA

^bDepartment of Mathematics, University of Beograd, Faculty of Mechanical Engineering, Kraljice Marije 16, 11120 Belgrade 35, Serbia

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 $[a, b] = \text{supp}(d\lambda)$. The n -point Gauss quadrature formula associated with $d\lambda$,

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

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, \dots , with respect to the inner product

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

2010 *Mathematics Subject Classification.* Primary 65D30; Secondary 65D32

Keywords. Rational averaged Gauss quadrature, Rational generalized averaged Gauss quadrature, Error estimations of rational Gauss quadrature

Received: 07 April 2020; Accepted: 18 April 2020

Communicated by Dragan S. Djordjević

The research of the first author was supported in part by NSF grants DMS-1720259 and DMS-1729509. The research of the second and the third authors was supported in part by the Serbian Ministry of Education, Science and Technological Development. Contract no. 451-03-68 / 2020-14 / 200105.

*Corresponding author

Email addresses: reichel@math.kent.edu (Lothar Reichel), mspalevic@mas.bg.ac.rs (Miodrag M. Spalević), jtomanovic@mas.bg.ac.rs (Jelena D. Tomanović)

They satisfy a three-term recurrence relation

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

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

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

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,

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

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 $\{\tau_v^G\}_{v=1}^n$ of the Gauss-Kronrod rule are the nodes of G_n . We refer to the remaining nodes, $\{\tau_{\mu}^K\}_{\mu=1}^{n+1}$, 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],

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

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

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

nodes $\{\tau_v^G\}_{v=1}^n$. 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

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

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

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

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

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

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

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

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

$$\int_{\mathbb{R}} p(t) d\tilde{\lambda}(t) = \sum_{v=1}^N \lambda_v f(\tau_v) \text{ for all } p \in \mathbb{P}_{d-1}, \tag{9}$$

Define

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

Then the quadrature formula (8) satisfies

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

with \mathfrak{S}_d defined by (7).

Conversely, if (8) and (11) hold with pairwise distinct nodes $\tilde{\tau}_\nu \in [a, b]$, 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 $\mathfrak{S}_{2n} = \mathbb{Q}_m \oplus \mathbb{P}_{2n-1-m}$. 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

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

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

$$\tilde{\tau}_\nu^G = \tau_\nu^G, \quad \tilde{\lambda}_\nu^G = \lambda_\nu^G \omega_m(\tau_\nu^G), \quad \nu = 1, 2, \dots, n,$$

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

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, $\mathfrak{S}_{3n+2} = \mathbb{Q}_m \oplus \mathbb{P}_{3n+1-m}$, 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

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

Its nodes and weights are given by

$$\tilde{\tau}_\nu^G = \tau_\nu^G, \quad \tilde{\tau}_\mu^K = \tau_\mu^K, \quad \tilde{\lambda}_\nu^{GK} = \lambda_\nu^{GK} \omega_m(\tau_\nu^G), \quad \tilde{\lambda}_\mu^K = \lambda_\mu^K \omega_m(\tau_\mu^K), \quad \nu = 1, 2, \dots, n, \quad \mu = 1, 2, \dots, n + 1,$$

where τ_ν^G and τ_μ^K are the nodes, while λ_ν^{GK} and λ_μ^K are the weights, of $(2n + 1)$ -point (polynomial) Gauss-Kronrod quadrature formula associated with the measure $d\tilde{\lambda} = d\lambda/\omega_m$.

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

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

We write the formulas for error estimation in the form

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

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

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

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 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 $m = 0, 2, \dots, 12$. 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	$ I - G_{n,m} $	$ I - K_{n,m} $	$ K_{n,m} - G_{n,m} $	$ I - L_{n,m} $	$ L_{n,m} - G_{n,m} $	$ I - S_{n,m} $	$ S_{n,m} - G_{n,m} $
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	$ I - G_{n,m} $	$ I - K_{n,m} $	$ K_{n,m} - G_{n,m} $	$ I - L_{n,m} $	$ L_{n,m} - G_{n,m} $	$ I - S_{n,m} $	$ S_{n,m} - G_{n,m} $
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	$G_{n,m}$	$ K_{n,m} - G_{n,m} $	$ L_{n,m} - G_{n,m} $	$ S_{n,m} - G_{n,m} $
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 $k \in \{\frac{1}{2}, \frac{3}{2}, \frac{5}{2}\}$. 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

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

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.

References

- [1] G.S. Ammar, D. Calvetti, L. Reichel, Computation of Gauss-Kronrod quadrature rules with non-positive weights, *Electron. Trans. Numer. Anal.* 9 (1999), 26–38.
- [2] D. Calvetti, G.H. Golub, W.B. Gragg, L. Reichel, Computation of Gauss-Kronrod quadrature rules, *Math. Comp.* 69 (2000), 1035–1052.
- [3] D.Lj. Djukić, L. Reichel, M.M. Spalević, Internality of generalized averaged Gaussian quadratures and their truncated variants for measures induced by Chebyshev polynomials, *Appl. Numer. Math.* 142 (2019), 190–205.
- [4] D.Lj. Djukić, L. Reichel, M.M. Spalević, J.D. Tomanović, Internality of generalized averaged Gauss rules and their truncations for Bernstein-Szegő weights, *Electron. Trans. Numer. Anal.* 45 (2016), 405–419.
- [5] D.Lj. Djukić, L. Reichel, M.M. Spalević, J.D. Tomanović, Internality of generalized averaged Gaussian quadrature rules and truncated variants for modified Chebyshev measures of the second kind, *J. Comput. Appl. Math.* 345 (2019), 70–85.
- [6] W. Gautschi, Gauss type quadrature rules for rational functions, *Intern. Ser. Numer. Math.* 112 (1993), 111–130.
- [7] W. Gautschi, On the computation of generalized Fermi-Dirac and Bose-Einstein integrals, *Comput. Phys. Commun.* 74 (1993), 223–238.
- [8] W. Gautschi, The use of rational functions in numerical quadrature, *J. Comput. Appl. Math.* 133 (2001), 111–126.
- [9] W. Gautschi, *Orthogonal Polynomials: Computation and Approximation*, Oxford University Press, Oxford, 2004.
- [10] W. Gautschi, OPQ: A MATLAB suite of programs for generating orthogonal polynomials and related quadrature rules (<http://www.cs.purdue.edu/archives/2001/wxg/codes>).
- [11] W. Gautschi, L. Gori, M.L. Lo Cascio, Quadrature rules for rational functions, *Numer. Math.* 86 (2000), 617–633.
- [12] G.H. Golub, J.H. Welsch, Calculation of Gauss quadrature rules, *Math. Comp.* 23 (1969), 221–230.
- [13] D.P. Laurie, Anti-Gaussian quadrature formulas, *Math. Comp.* 65 (1996), 739–747.
- [14] D.P. Laurie, Calculation of Gauss-Kronrod quadrature rules, *Math. Comp.* 66 (1997), 1133–1145.
- [15] G.V. Milovanović, M.M. Spalević, M.S. Pranić, On the remainder term of Gauss-Radau quadratures for analytic functions, *J. Comput. Appl. Math.* 218 (2008), 281–289.
- [16] G.V. Milovanović, M.M. Spalević, M.S. Pranić, Error estimates for Gauss-Turán quadratures and their Kronrod extensions, *IMA J. Numer. Anal.* 29 (2009), 486–507.
- [17] G.V. Milovanović, M.M. Spalević, M.S. Pranić, Error estimates for Gaussian quadratures for analytic functions, *J. Comput. Appl. Math.* 233 (2009), 802–807.
- [18] S.E. Notaris, Gauss-Kronrod quadrature formulae - A survey of fifty years of research, *Electron. Trans. Numer. Anal.* 45 (2016), 371–404.
- [19] S.E. Notaris, Stieltjes polynomials and related quadrature formulae for a class of weight functions, II, *Numer. Math.* 142 (2019), 129–147.
- [20] F. Peherstorfer, On positive quadrature formulas, *Intern. Ser. Numer. Math.* 112 (1993), 297–313.
- [21] M.M. Spalević, On generalized averaged Gaussian formulas, *Math. Comp.* 76 (2007), 1483–1492.
- [22] M.M. Spalević, A note on generalized averaged Gaussian formulas, *Numer. Algor.* 46 (2007), 253–264.
- [23] M.M. Spalević, On generalized averaged Gaussian formulas. II, *Math. Comp.* 86 (2017), 1877–1885.
- [24] M.M. Spalević, A note on generalized averaged Gaussian formulas for a class of weight functions, *Numer. Algor.* 85 (2020), 977–993.