Quadrature Rules Based on Partial Fraction Expansions

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Quadrature rules are typically derived by requiring that all polynomials of a certain degree be integrated exactly. The nonstandard issue discussed here is the requirement that, in addition to the polynomials, the rule also integrates a set of prescribed rational functions exactly. Recurrence formulas for computing such quadrature rules are derived. In addition, Fejér's first rule, which is based on polynomial interpolation at Chebyshev nodes, is extended to integrate also rational functions with pre-assigned poles exactly. Numerical results, showing a favorable comparison with similar rules that have been proposed in the literature, are presented. An error analysis of a representative test problem is given.

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1. Introduction

Classical quadrature rules, whether of interpolatory or Gaussian type, are designed to integrate all polynomials of a given degree exactly. These methods work well if the integrand is polynomial-like in the sense that there are no singularities in the finite complex plane, or if singularities do exist that they be far from the interval under consideration. To be able to handle the situation where there is a finite number of isolated poles close to the interval, research emphasis has recently shifted to quadrature rules that integrate not only polynomials exactly, but also rational functions with prescribed poles (see [2], [4], [6], [11]).

In this paper we therefore consider quadrature formulas

$$\int_{-1}^{1} f(x)\,dx \approx \sum_{j=1}^{N} w_j f(x_j) \tag{1}$$

that are exact for partial fraction expansions of the form

$$f(x) = \sum_{j=0}^{K-1} a_j x^j + \sum_{j=1}^{M} \frac{b_j}{x - z_j}. \tag{2}$$

The poles $\{z_j\}_{j=1}^{M} \in \mathbb{C}/[-1,1]$ will be pre-assigned. The following two classes of quadrature rules of this type will be distinguished:

Class I (Interpolatory) Both the nodes $\{x_j\}_{j=1}^{N} \in [-1,1]$ and the poles $\{z_j\}_{j=1}^{M} \in \mathbb{C}/[-1,1]$ are fixed. Only the weights $\{w_j\}_{j=1}^{N}$ in (1) are to be determined. This rule is exact for polynomials of degree less than $K = N - M$. It is assumed that $M \leq N$; if $M = N$ the first sum in (2) is void and the rule is exact only for the rational functions.

Class G (Gaussian) Only the poles $\{z_j\}_{j=1}^{M} \in \mathbb{C}/[-1,1]$ are fixed. Both the nodes $\{x_j\}_{j=1}^{N}$ and the weights $\{w_j\}_{j=1}^{N}$ need to be determined. With the N additional degrees of freedom (i.e., the nodes) the polynomial degree of the rule can be increased to $K = 2N - M$. As before the prescribed M rational functions are also to be integrated exactly.

In the case $M = 0$ (i.e., polynomials only, no rational functions) it may be shown that the method in class Class G is unique, which is of course the well-known Gauss-Legendre rule. The nodes $\{x_j\}_{j=1}^{N}$ turn out to be the roots of the Legendre polynomial of degree N, and the weights can be computed explicitly (see [3, p. 97]). On the other hand, several methods in Class I ($M = 0$) have been proposed. These rules, which are distinguished only by their choice of nodes

$\{x_j\}_{j=1}^N$, are associated with the names of Basu, Clenshaw and Curtis, and Fejér (see [3, p. 84]).

We shall be particularly interested in Fejér's first rule. The nodes are chosen as the roots of the Chebyshev polynomial of degree N, i.e.,

$$x_j = \cos\theta_j, \qquad \theta_j = \frac{(2j-1)\pi}{2N}, \qquad j = 1, \ldots, N. \tag{3}$$

When $M = 0$ the corresponding weights can be computed explicitly (see [3, p. 85])

$$w_j = \frac{2}{N}\left\{1 - 2\sum_{k=1}^{[N/2]} \frac{\cos(2k\theta_j)}{4k^2-1}\right\}. \tag{4}$$

The present paper has two objectives. First, we extend Fejér's first rule to the case $M \geq 1$. Second, we present a new recursive algorithm for computing the quadrature rules in both classes I and G.

The case $M \geq 1$ has been considered to a limited degree in the literature. Methods in Class I have been introduced, for example, in [2] and [6]. In these papers the poles $\{z_j\}_{j=1}^M$ are chosen generically and are not matched to the poles of the integrand. The present paper takes a different view: We assume that the integrand $f(x)$ is meromorphic in a domain containing $[-1,1]$ and that the locations of the poles are known. The poles $\{z_j\}_{j=1}^M$ in (2) are then selected to coincide with the poles of $f(x)$ nearest the interval $[-1,1]$. This, as we shall see, effectively makes the integrand analytic in a wide region about $[-1,1]$ and the quadrature rule converges quickly. This method, when based on the Chebyshev nodes (3), will be referred to as the Rational Fejér Rule.

Methods in Class G, with $M \geq 1$, have been considered in [4] and [11], for example, and algorithms for the generation of these rules have been presented in [5]. The method discussed here, which will be referred to as the Rational Gauss Rule, is essentially equivalent to the method introduced in [4] and one of the methods discussed in [11]. The way in which the quadrature rule is generated here, however, is fundamentally different from the algorithms presented in [5].

The outline of the paper is as follows: In the next section we take a closer look at the Rational Fejér and Gauss Rules alluded to above. Section 3 is devoted to the computational details of constructing these rules. In Section 4 the two rules will be compared numerically. A representative test example will be analyzed in Section 5 to establish the rate of convergence of the Rational Fejér Rule.

2. The Rational Fejér and Rational Gauss Rules

We start this section with the Rational Fejér Rule, which is defined as the quadrature rule (1) that is exact for the partial fraction expansion (2), with $K = N - M$. The nodes $\{x_j\}_{j=1}^{N}$ are the Chebyshev points (3). The prescribed poles $\{z_j\}_{j=1}^{M} \in \mathbb{C}/[-1, 1]$ will be assumed distinct. If they are complex, they should occur in conjugate pairs to guarantee that the weights are real.

The direct way of computing the weights of this rule is to require exactness of the quadrature rule (1) for (a) the monomials x^k, $k = 0, \ldots, N - M - 1$, and (b) the rational functions $1/(x - z_k)$, $k = 1, \ldots, M$. This leads to an $N \times N$ mixed Vandermonde-Cauchy linear system for solving the w_j. This system is typically ill-conditioned, however, and does not represent a practical method for solving the problem.

Instead, we note that the partial fraction expansion (2) can be represented as the rational function

$$f(x) = \frac{\sum_{j=0}^{N-1} c_j x^j}{\prod_{j=1}^{M}(x - z_j)} = \frac{\sum_{j=0}^{N-1} d_j T_j(x)}{\prod_{j=1}^{M}(x - z_j)},$$

where $T_j(x)$ is the Chebyshev polynomial of degree j. It is therefore sufficient to require exactness of the rule (1) for the functions

$$f(x) = \frac{T_k(x)}{q(x)}, \qquad k = 0, \ldots, N - 1,$$

where

$$q(x) = (x - z_1)(x - z_2) \ldots (x - z_M). \tag{5}$$

(Note that because of the restrictions on the poles mentioned above, $q(x)$ is a polynomial with real coefficients.) This requirement leads to the linear system

$$\sum_{j=1}^{N} w_j \frac{T_k(x_j)}{q(x_j)} = \int_{-1}^{1} \frac{T_k(x)}{q(x)}\, dx, \qquad k = 0, \ldots, N - 1, \tag{6}$$

which may be solved by making use of the discrete orthogonality properties of the Chebyshev polynomials. The solution is

$$w_j = \frac{2}{N} q(x_j) \left\{ \frac{1}{2}\mu_0 + \sum_{k=1}^{N-1} \cos(k\theta_j)\mu_k \right\}, \qquad j = 1, \ldots, N, \tag{7}$$

where we have defined the modified moments μ_k by

$$\mu_k = \int_{-1}^{1} \frac{T_k(x)}{q(x)}\, dx, \qquad k = 0, \ldots, N-1. \tag{8}$$

The ill-conditioned Vandermonde-Cauchy system alluded to above has been replaced by the well-conditioned (essentially orthogonal) Chebyshev system (6). The tradeoff is that one now requires a method for the efficient computation of the moments μ_k. This is the topic of the next section.

Observe that if $q(x) \equiv 1$ (i.e., $M = 0$) the μ_k may be evaluated explicitly by the formula

$$\int_{-1}^{1} T_k(x)\, dx = \begin{cases} 0 & k \text{ odd} \\ \frac{2}{1-k^2} & k \text{ even.} \end{cases} \tag{9}$$

In this case it is easy to check that formula (7) reproduces the weights of Fejér's first rule (4).

We now derive the Rational Fejér Rule from a different angle, which will be useful in the error estimates of Section 5, and will also lead to an alternative expression for the weights (7). Let $q(x)$ be defined by (5), and interpolate the function $f(x)q(x)$ by a polynomial $p_{N-1}(x)$ of degree $N-1$ at the Chebyshev points (3). Then the rational $(N-1, M)$ approximation to $f(x)$ with the pre-assigned poles $\{z_j\}_{j=1}^{M}$ is given by

$$f(x) \approx \frac{p_{N-1}(x)}{q(x)}. \tag{10}$$

The Rational Fejér Rule is equivalent to integrating the right-hand side exactly.

Observe that if the zeros of $q(x)$ are chosen to annihilate the M poles of $f(x)$ nearest to $[-1,1]$, the function $f(x)q(x)$ becomes analytic in a wide region containing this interval. The wider the region of analyticity, the quicker the convergence of the polynomial interpolation process (see [8, Sect. 12.2]). This explains the high accuracy of the Rational Fejér Rule that will be observed empirically in Section 4, and which will be analyzed theoretically in Section 5.

The alternative expression for the weights alluded to above is obtained by following the procedure sketched in [8, Sect. 6.1] for polynomial based rules. Consider the Lagrange form of the interpolant, i.e.,

$$p_{N-1}(x) = \sum_{j=1}^{N} \frac{T_N(x)}{T_N'(x_j)(x - x_j)} f(x_j) q(x_j). \tag{11}$$

Dividing by $q(x)$ and integrating both sides on $[-1,1]$ yields the following expression for the weights as alternative to (7)

$$w_j = \frac{q(x_j)}{T_N'(x_j)} \int_{-1}^{1} \frac{T_N(x)}{q(x)(x-x_j)}\, dx, \qquad j = 1,\ldots,N. \tag{12}$$

As the integrand is a rational function, the integral can be evaluated by partial fractions. For example, when $M = N$ a quick computation yields

$$w_j = \frac{q(x_j)}{T_N'(x_j)} \sum_{k=1}^{M} \frac{T_N(z_k)}{q'(z_k)} \frac{\eta_k}{z_k - x_j}, \qquad j = 1,\ldots,N, \tag{13}$$

where the η_k are defined by

$$\eta_k = \int_{-1}^{1} \frac{dx}{x - z_k} = \log\left(\frac{z_k - 1}{z_k + 1}\right). \tag{14}$$

Summing series such as (13) does not seem to be a practical method for computing the weights, at least not in standard floating-point arithmetic. This is due to the fact that the terms are typically large and of mixed sign, so severe cancellation occurs. (We have tried most of the special techniques for floating-point summation described in [7], for example, without success.) In our computer implementation we have computed the weights according to (7).

Whereas the weights of Fejér's first rule, defined by (4), are all positive, this need not be the case for the weights of the Rational Fejér Rule defined by (7). Neither formula (7) nor formula (12) seem to offer a straightforward criterion to decide a priori whether a given choice of poles $\{z_j\}_{j=1}^{M}$ will yield positive weights or not. Numerical experiments have indicated that: (a) If the set of poles $\{z_j\}_{j=1}^{M}$ is fixed and N is sufficiently large, then all w_j are positive, and (b) if the poles are real and symmetric with respect to the origin, then all w_j are positive even if $M \propto N$. We will encounter the latter situation in the numerical test in Section 4 below.

Turning to the Rational Gauss Rule, we observe that the moments (8) may also be used to construct rules in this class. We wish to find polynomials orthogonal on $[-1,1]$ with respect to the rational weight $1/q(x)$, where $q(x)$ is defined by (5). This is a classical problem in Gaussian quadrature and we merely sketch the details. (For more details, see [3] for example.)

An algorithm for generating orthogonal polynomials for arbitrary weights has been developed in [10] and [12]. This algorithm requires as input the modified moments (8), for $k = 0,\ldots,2N-1$. The output gives the coefficients of the three-term recurrence that defines these orthogonal polynomials. Once the recurrence coefficients are available, the nodes of the quadrature rule may be obtained by computing the eigenvalues of the associated Jacobi matrix. The weights are computed as the squares of the leading components of the normalized eigenvectors.

Under the restrictions we have placed on the poles (single multiplicity, complex poles occurring in conjugate pairs) the weight function $1/q(x)$ is real-valued and nonzero on $[-1,1]$. In this case standard Gaussian quadrature theory predicts that all weights are positive, and that all nodes lie in the interval of support $[-1,1]$ (see [3, Sect. 2.7]).

3. Recurrence Formulas for the Modified Moments

In the previous section we observed that once sufficiently many modified moments (8) have been computed, it is straightforward to compute both the Rational Fejér and Rational Gauss Rules. We therefore turn to the computation of these quantities, for which we derive recursive algorithms that are similar in spirit to the ones given in [1]. What is described next applies to Fejér formulae; for Gauss formulae one would have to replace N by $2N-1$.

Let $q_0(x) \equiv 1$ and define, for $j = 1, \ldots, M$,

$$q_j(x) = (x - z_1)(x - z_2)\ldots(x - z_j).$$

Define further, for $j = 1, \ldots, M$ and $k = 0, \ldots, N-1$,

$$m_{k,j} = \int_{-1}^{1} \frac{T_k(x)}{q_j(x)}\, dx. \tag{15}$$

The modified moments (8) that we wish to compute are determined by

$$\mu_k = m_{k,M}.$$

By using the well-known three-term recurrence relation for Chebyshev polynomials one obtains, for $j = 1, \ldots, M$ and $k = 1, \ldots, N-1$,

$$\begin{aligned}\int_{-1}^{1} \frac{T_k(x)}{q_j(x)}\, dx &= \int_{-1}^{1} \frac{2xT_{k-1}(x) - T_{k-2}(x)}{q_j(x)}\, dx,\\ &= \int_{-1}^{1} \frac{2(x-z_j)T_{k-1}(x) + 2z_jT_{k-1}(x) - T_{k-2}(x)}{q_j(x)}\, dx,\end{aligned}$$

which yields the two-dimensional recurrence

$$m_{k,j} = 2m_{k-1,j-1} + 2z_j m_{k-1,j} - m_{k-2,j}.$$

(Here it is understood that $m_{-1,j} = 0$ for $j = 1, \ldots, M$.)

For implementation purposes we rewrite this recurrence as

$$m_{k,j} - 2z_j m_{k-1,j} + m_{k-2,j} = 2m_{k-1,j-1}, \tag{16}$$

the computational stencil of which is shown in Figure 1(b). With j fixed this is a non-homogeneous second-order linear difference equation in k, where the right-hand side has been computed at the previous j-level. The starting values ($j = 0$) are provided by

$$m_{k,0} = \int_{-1}^{1} T_k(x)\, dx, \tag{17}$$

which may be evaluated by (9). Two boundary values ($k = 0$, $k = \infty$) are given by

$$m_{0,j} = \int_{-1}^{1} \frac{dx}{q_j(x)}, \qquad \lim_{k\to\infty} m_{k,j} = 0, \tag{18}$$

for each $j = 1, \ldots, M$. The latter formula follows from the fact that for each j, the quantity $m_{k,j}$ is nothing but the k-th Chebyshev coefficient of the function $(\pi/2)\sqrt{1-x^2}/q_j(x)$, which is continuous on $[-1, 1]$. The boundary values $m_{0,j}$ defined by the integral in (18) may be computed by another recursion, the details of which will be given below.

The recurrence (16) may be implemented explicitly, by making use of $m_{0,j}$ defined by (18), and

$$m_{1,j} = \int_{-1}^{1} \frac{x}{q_j(x)}\, dx$$

as initial values. In the computational stencil shown in Figure 1(b), the black and white dots indicate, respectively, known and unknown quantities. The matrix of moments $m_{k,j}$ may therefore be completed in a column-by-column (or row-by-row) order. However, this implementation is numerically unstable. The solution of the homogeneous version of (16) consists of the two modes $\left(z_j \pm \sqrt{z_j^2 - 1}\right)^k$ (with j-fixed). The only way both these modes will be bounded as $k \longrightarrow \infty$ is when $z_j \in [-1, 1]$, which is not allowed in the current setting. Therefore, if $z_j \in \mathbb{C}/[-1, 1]$, any roundoff error made in the computation of the initial values will be amplified exponentially as k increases.

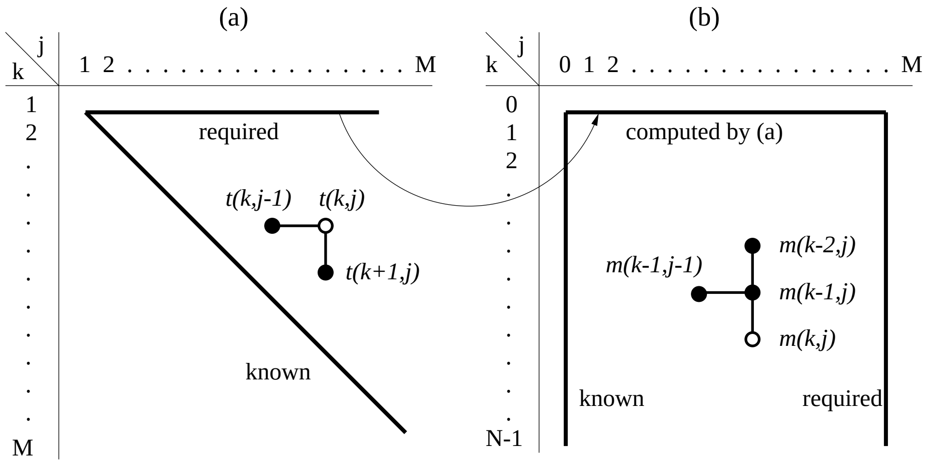

Figure 1. Computational stencils of (a) the initializing recurrence (21), and (b) the main recurrence (16).

The correct approach, as indicated by J.C.P. Miller and others, is to view (16) not as an initial value problem but rather as a boundary value problem. For each j, the recurrence is treated as a tridiagonal linear system, the solution of which determines the quantities $m_{k,j}$, $k = 0, \ldots, N-1$ implicitly. To implement this the second boundary condition in (18) needs to be approximated. One way of doing this is to asymptotically estimate the integral (15) in the limit $k \longrightarrow \infty$, j-fixed. Alternatively, one can impose the artificial boundary condition

$$m_{L,j} = 0,$$

for L some integer greater than $N-1$, typically $L \gg N$.

There exists a special tridiagonal solver due to F.W.J. Olver [9], which relieves the user of the burden of determining an appropriate value of L by trial-and-error. This algorithm provides a fast and automatic way to determine a value L such that, for a given tolerance ϵ,

$$|m_{k,j}^{(L)} - m_{k,j}^{(L+1)}| \leq \epsilon, \qquad k = 0, 1, \ldots, N-1.$$

Here $m_{k,j}^{(L)}$ and $m_{k,j}^{(L+1)}$ represent the solution of (16) with boundary conditions $m_{L,j} = 0$ and $m_{L+1,j} = 0$ respectively.

A few practical matters deserve pointing out. As the $m_{k,j}$ may be large (or small) we found it necessary to replace the absolute stopping criterion above, by the relative test

$$\left| \frac{m_{k,j}^{(L)} - m_{k,j}^{(L+1)}}{m_{0,j}} \right| \leq \epsilon, \qquad k = 0, 1, \ldots, N-1. \tag{19}$$

Also, if z_j is close to the interval $[-1, 1]$ then L is large, whereas $L \approx N$ when $|z_j|$ is large. Thus a judicious ordering of the poles z_j is required to ensure that enough moments at the previous j-level have been computed to provide the full right-hand side of (16). For example, in the test examples in Section 4 below the poles will either be real or pure imaginary. In both cases they should be indexed such that $|z_1| \leq |z_2| \leq \ldots \leq |z_M|$. We have not yet explored the situation in which some poles are real and others are complex.

It remains to discuss the computation of the first boundary condition in (18), namely

$$m_{0,j} = \int_{-1}^{1} \frac{dx}{q_j(x)}. \tag{20}$$

Define, for each integer $k \leq j$,

$$t_{k,j} = \int_{-1}^{1} \frac{dx}{(x - z_k)(x - z_{k+1}) \ldots (x - z_j)}.$$

The boundary values (20) that we wish to compute are determined by

$$m_{0,j} = t_{1,j}, \qquad j = 1, \ldots, M.$$

A quick calculation yields

$$t_{k+1,j} - t_{k,j-1} = \int_{-1}^{1} \left(\frac{1}{\prod_{\ell=k+1}^{j}(x - z_\ell)} - \frac{1}{\prod_{\ell=k}^{j-1}(x - z_\ell)} \right) dx = (z_j - z_k) t_{k,j},$$

and hence

$$t_{k,j} = \frac{t_{k+1,j} - t_{k,j-1}}{z_j - z_k}. \tag{21}$$

This is another two-dimensional recurrence, the computational stencil of which is shown in Figure 1(a). As before the black/white dots indicate known/unknown quantities. The recurrence can therefore be implemented explicitly, by completing the upper triangular part of the matrix $t_{k,j}$, in a diagonal-by-diagonal manner starting with the main diagonal $t_{j,j}$, which consists of the known quantities

$$t_{j,j} = \int_{-1}^{1} \frac{dx}{x - z_j} = \eta_j, \qquad j = 1, \ldots, M. \tag{22}$$

The η_j are defined by (14).

In summary, Figure 1 shows a schematic representation of our algorithm for computing the modified moments μ_k defined by (8). It consists of two recurrences: (a) the initializing recurrence, and (b) the main recurrence. The initializing recurrence (21) is used to compute the upper-triangular matrix $t_{k,j}$ in a diagonal-by-diagonal manner starting with known quantities on the main diagonal. Once $t_{1,j}$ have been computed for $j = 1, \ldots, M$, these values become the boundary values $m_{0,j}$ for the main recurrence (16). This recurrence is used to compute the matrix $m_{k,j}$ in a column-by-column manner, by solving for $m_{k,j}$, $k = 0, \ldots, N-1$ at each j-level, starting with $j = 1$ and terminating at $j = M$. Once the M-th column is reached, the quantities $m_{k,M}$ provide the modified moments μ_k, $k = 0, \ldots, N-1$.

4. Numerical Tests

Following [4], we consider the test example

$$I(\omega) = \int_{-1}^{1} \frac{\pi x/\omega}{\sin(\pi x/\omega)}\, dx, \qquad \omega > 1. \tag{23}$$

When $\omega \approx 1$ the integrand resembles a square well, with almost flat bottom at $y \approx 1$ for most of the interval, and steep sides reaching to a maximum of $y = (\pi/\omega)/\sin(\pi/\omega) \approx 1/(\omega - 1)$ at $x = \pm 1$. As we shall see, the large gradients near the endpoints cause problems for quadrature rules based on polynomials.

By contrast, the integrand, being meromorphic, is tailor-made for the methods based on rational functions. It has poles at $\pm\omega$, $\pm 2\omega$, ..., and so we choose, for an even integer M,

$$z_j = (-1)^j \lfloor (j+1)/2 \rfloor \omega, \qquad j = 1, \ldots, M. \tag{24}$$

We have applied both the Rational Fejér and Rational Gauss Rules to this integral, as well as standard Gauss-Legendre quadrature and Fejér's first rule. (In [4] and [5] similar computations were presented, but these did not include the Fejér rules.) Figure 2 shows the relative errors, on a log-scale, versus N, the number of points in the rule, when $\omega = 1.001$. (The reference value of $I(1.001)$ was obtained by a high-precision computation in Maple.) It turned out that there was very little difference between the Gauss-Legendre rule and Fejér's first rule, at least for $N \leq 20$, so to avoid clutter we decided not to display the Fejér error curve.

The algorithm described in the previous section was used to construct both the Rational Fejér and Rational Gauss Rules. For the Rational Fejér Rule we have picked $M = N$, i.e., the rule is exact for the M rational functions with poles given by (24), and no polynomials. The weights were found to be positive for all $N = 2, 4, \ldots, 20$. In the Rational Gauss Rule we have picked $M = 2N$, which likewise means that the rule is exact for the prescribed rational functions only. The relative tolerance in Olver's algorithm (cf. 19) was set to $\epsilon = 10^{-14}$, an arbitrary choice. (The computations were done in MATLAB, with machine epsilon equal to about 2.22×10^{-16}.)

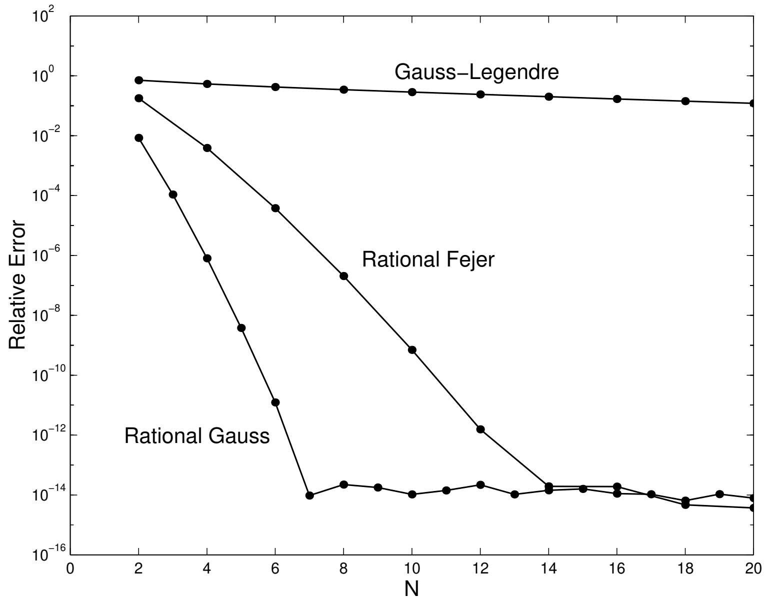

Figure 2. Relative error in the Gauss-Legendre Rule, Rational Fejér Rule (with $M = N$), and Rational Gauss Rule (with $M = 2N$). The test problem is $I(1.001)$ defined by (23).

As was predicted above, the polynomial based Gauss-Legendre rule and Fejér's first rule both converge slowly. (It may be deduced from the results of Section 5 below that the convergence rate of Fejér's first rule is essentially

$O((\omega+\sqrt{\omega^2-1})^{-N}) \approx O(0.96^N))$. By contrast, both methods based on rational functions converge quickly, at rates that appear to be faster than geometric. We analyze this speed of convergence in Section 5 below.

It is no surprise that the Rational Gauss Rule is superior to the Rational Fejér Rule, as for each N it integrates twice as many rational functions exactly. On the other hand, it is more expensive to compute the Rational Gauss Rule. First, the construction of the N point Rational Gauss Rule requires $2N$ modified moments, compared to the N for the Rational Fejér Rule. Second, the computation of the nodes and weights of the Rational Gauss Rule requires that all roots of an N-th degree polynomial be calculated, compared to the Rational Fejér Rule for which the nodes and weights are given explicitly (by (3) and (7) respectively).

We feel it is appropriate to include the operation count for the construction of the rule when two quadrature rules based on rational functions are compared. The weights and nodes of polynomial based rules may be constructed once and for all, but this is not the case for the methods discussed here. To achieve optimal accuracy in both the Rational Fejér and Rational Gauss Rules one needs to match the poles of the partial fraction expansion (2) to the poles of the integrand. Therefore each new integral requires a new rule to be constructed. When these considerations are taken into account, it appears as if the Rational Fejér Rule might be a worthy competitor to the Rational Gauss Rule.

An anonymous referee suggested that we should also include in these comparisons the well-known strategy of subtracting singularities. In the case of the integral (23) this amounts to adding $2\omega^2/(x^2-\omega^2)$ to the integrand, which eliminates the poles at $\pm\omega$; see (26) below. The standard Gauss-Legendre rule, for example, may now be applied to the modified integrand. This strategy does indeed work well—its error curve lies somewhere between the error curves of the Fejér and Gauss rules seen in Figure 2. Its convergence rate is geometric, however, in contrast to the other two rules which converge at a super-geometric rate. If the computations of Figure 2 were to be repeated in quadruple precision, the suggested method will almost surely end up less accurate than the Rational Fejér rule for some N sufficiently large. Moreover, the suggested method requires the location of the poles as well as the corresponding residues as input. The Rational Fejér and Gauss rules do not require residue information.

As a second test we applied these rules to the integral

$$J(\omega) = \int_{-1}^{1} \frac{\pi x/\omega}{\sinh(\pi x/\omega)}\, dx, \qquad \omega > 0. \tag{25}$$

Now the integrand exhibits a narrow peak centered at the origin when $\omega \approx 0$. The poles are pure imaginary and the parameters $\{z_j\}_{j=1}^{M}$ were chosen as in (24) but multiplied by i (the complex unit).

We constructed both the Rational Fejér and Rational Gauss Rules by the algorithm described in Section 3, with relative error tolerance $\epsilon = 10^{-14}$ in (19). As in Figure 2 we used $M = N$ for the Rational Fejér Rule, and $M = 2N$ for the Rational Gauss Rule. The tridiagonal system (16) was solved using complex arithmetic, a convenient feature of MATLAB.

With $\omega = 0.1$ the error curves were qualitatively similar to the curves shown in Figure 2, and therefore they are not reproduced here. Again the polynomial based methods were distinctly inferior to their rational counterparts, and the Rational Gauss Rule was superior to the Rational Fejér Rule. The convergence rates of both the Rational Fejér and Rational Gauss Rules, though still faster than geometric, were not as rapid as in Figure 2 however. The Rational Fejér Rule reached the relative tolerance of 10^{-14} only at $N \approx 34$, compared to the $N \approx 14$ seen in Figure 2. For the Rational Gauss Rule these numbers were $N \approx 20$ vs. $N \approx 7$. In this experiment the Rational Fejér Rule turned out to have some negative weights, although not sufficiently large in magnitude to have a detrimental effect on the quality of the approximation.

We report that when ω was reduced to below 0.1, both the Rational Fejér and Rational Gauss Rules showed signs of instability when approximating (25). The Rational Fejér Rule produced weights that were large and of mixed sign, so severe cancellation occurred. In some cases the Rational Gauss Rule became degenerate, in that some of its nodes appeared to coalesce at the origin. Relatedly, the Olver algorithm had difficulty in reaching the error tolerance (19) for both rules. These difficulties will be addressed in future work.

5. Rate of Convergence: An Example

Convergence proofs for methods in CLASS I ($M \geq 1$) and CLASS G ($M \geq 1$) have been presented in [2], [6] and [11] respectively. The error estimates presented in these references are very general, and therefore they lack a certain degree of sharpness. Here we shall do the opposite: we sacrifice generality in exchange for tight and explicitly computable bounds.

We restrict ourselves to the specific integral (23), which we consider to be a model problem for the class of integrals involving meromorphic functions. The aim is to make clear the super-fast rate of convergence observed in Figure 2. We believe that the convergence analysis presented here will also be applicable to other integrals in this class, but such generalizations will be pursued elsewhere.

Only the Rational Fejér Rule is considered here. This rule is easier to analyze than the Rational Gauss Rule, since the nodes are known a priori. It is therefore possible to bound the interpolation error, from which the quadrature error follows directly.

We consider therefore the integral (23), and apply the well-known partial fraction expansion of the co-secant to the integrand. This yields

$$f(x) = \frac{\pi x/\omega}{\sin(\pi x/\omega)} = 1 - 2x^2 \left\{ \frac{1}{x^2-\omega^2} - \frac{1}{x^2-4\omega^2} + \frac{1}{x^2-9\omega^2} - \dots \right\}, \tag{26}$$

where $\omega > 1$. Let $q(x)$ be defined by (5), with the choice of poles given by (24). That is, with M assumed to be even,

$$q_M(x) = (x^2-\omega^2)(x^2-4\omega^2)\dots(x^2-(\tfrac{1}{2}M)^2\omega^2). \tag{27}$$

We have added the subscript to stress the fact that this is a polynomial of degree M.

The following two Lemmas will be useful:

Lemma 1. With $f(x)$ and $q_M(x)$ defined by (26) and (27), it follows that for each $x \in [-1,1]$,

$$\left| \frac{q_M((\frac{1}{2}M+1)\omega)}{f(x)q_M(x)} \right| \le \binom{M+1}{\frac{1}{2}M+1}.$$

Proof. By using the well-known infinite product representation of $\sin x/x$ it follows that

$$f(x)q_M(x) = \frac{(x^2-\omega^2)(x^2-4\omega^2)\dots(x^2-(\frac{1}{2}M)^2\omega^2)}{\left(1-\frac{x^2}{\omega^2}\right)\left(1-\frac{x^2}{4\omega^2}\right)\left(1-\frac{x^2}{9\omega^2}\right)\dots}.$$

By cancelling the first $\frac{1}{2}M$ factors one obtains, for each $x \in [-1,1]$,

$$|f(x)q_M(x)| \ge (\tfrac{1}{2}M)!^2\omega^M$$

(with equality at $x=0$). A direct calculation shows that

$$q_M((\tfrac{1}{2}M+1)\omega) = \frac{(M+1)!}{\frac{1}{2}M+1}\omega^M.$$

Taking the ratio of these two expressions yields the required inequality. $\square$

Lemma 2. Let $p_{N-1}(x)$ be the polynomial interpolant of degree $N-1$ of the function

$$f(x) = \frac{1}{x^2 - a^2}, \qquad a > 1,$$

at the Chebyshev nodes $\{x_j\}_{j=1}^N$ defined by (3). Then the pointwise error on $[-1,1]$ is given by

$$\frac{1}{x^2-a^2} - p_{N-1}(x) = \frac{1}{x^2-a^2}\frac{T_N(x)}{T_N(a)} \times \begin{cases} 1 & N \text{ even} \\ x/a & N \text{ odd.} \end{cases}$$

Proof. The Hermite formula for the error in polynomial interpolation at Chebyshev nodes is given by the contour integral [8, p. 245]

$$f(x) - p_{N-1}(x) = \frac{1}{2\pi i}\int_C \frac{T_N(x)}{T_N(z)}\frac{f(z)}{z-x}\,dz.$$

Here C is any simple closed rectifiable curve that contains the interval $[-1,1]$. The function $f(z)$ is assumed to be analytic in a region that contains C, which means that the points $z = \pm a$ should not be enclosed by C. By Cauchy's Theorem it is permissible to deform the contour C into the circle $|z| = R$, $R > a$, provided one subtracts the residue contributions of the poles at $z = \pm a$. Hence

$$f(x) - p_{N-1}(x) = \frac{1}{2\pi i}\int_{|z|=R} \frac{T_N(x)}{T_N(z)}\frac{dz}{(z^2-a^2)(z-x)} - \text{Res}(z=a) - \text{Res}(z=-a).$$

It is a standard exercise in complex analysis to show that the integral on the right vanishes in the limit $R \longrightarrow \infty$. By computing the residues directly,

$$f(x) - p_{N-1}(x) = -\frac{1}{2a}\frac{T_N(x)}{T_N(a)}\frac{1}{a-x} - \frac{1}{2a}\frac{T_N(x)}{T_N(-a)}\frac{1}{a+x},$$

from which the result follows. $\square$

Having disposed of the auxilliary results we are now in a position to compute the error in the rational approximation (10). This is given in the following proposition.

Proposition 3. Let $f(x)$, $q_M(x)$, and $p_{N-1}(x)$ be defined by (26), (27), and (11), respectively. If $N > M$, it follows that for each $x \in [-1,1]$,

$$f(x) - \frac{p_{N-1}(x)}{q_M(x)} = 2\frac{T_N(x)}{q_M(x)} \sum_{k=\frac{1}{2}M+1}^{\infty} (-1)^k \frac{q_M(k\omega)}{T_N(k\omega)}\frac{\psi_k}{x^2-k^2\omega^2}, \tag{28}$$

where

$$\psi_k = \begin{cases} k^2\omega^2 & N \text{ even} \\ k\omega x & N \text{ odd.} \end{cases}$$

Proof. From (26), (27) it follows that

$$f(x)q_M(x) = (\text{polynomial of degree} \le M) + (-1)^{\frac{1}{2}M+1} 2x^2 \times \left\{ \frac{q_M(x)}{x^2-(\frac{1}{2}M+1)^2\omega^2} - \frac{q_M(x)}{x^2-(\frac{1}{2}M+2)^2\omega^2} + \frac{q_M(x)}{x^2-(\frac{1}{2}M+3)^2\omega^2} - \dots \right\}.$$

Since M is even, each rational function inside the braces may be expressed as

$$\frac{q_M(x)}{x^2-a^2} = p_{M-2}(x) + \frac{q_M(a)}{x^2-a^2},$$

for some polynomial $p_{M-2}(x)$ of degree at most $M-2$. Therefore,

$$f(x)q_M(x) = (\text{polynomial of degree} \le M) + (-1)^{\frac{1}{2}M+1} 2x^2 \times \left\{ \frac{q_M((\frac{1}{2}M+1)\omega)}{x^2-(\frac{1}{2}M+1)^2\omega^2} - \frac{q_M((\frac{1}{2}M+2)\omega)}{x^2-(\frac{1}{2}M+2)^2\omega^2} + \frac{q_M((\frac{1}{2}M+3)\omega)}{x^2-(\frac{1}{2}M+3)^2\omega^2} - \dots \right\}.$$

Since $N > M$ was assumed, polynomial interpolation of degree $N-1$ will be exact for the polynomial part of the right-hand side. Therefore only the error in the rational part needs to be computed. This may be accomplished with the aid of Lemma 2, as each rational function on the right is of the form

$$\frac{x^2}{x^2-a^2} = 1 + \frac{a^2}{x^2-a^2}.$$

$\square$

Remark 4. The proof of the above proposition does not carry over, without modification, to the case $N = M$. We have not pursued such modifications, but we investigated numerically and it appears that the error bound (29) below might also be valid when $N = M$.

By using Proposition 3 the following uniform bound for the relative error in the rational approximation (10) is obtained. (Note that we estimate the relative error, as the absolute error is of little use due to the large values of $f(x)$ on $[-1,1]$ when $\omega \approx 1$.)

Theorem 5. Under the assumptions of Proposition 3 it follows that for each $x \in [-1,1]$,

$$\left| \frac{f(x) - \frac{p_{N-1}(x)}{q_M(x)}}{f(x)} \right| \leq B(M,N,\omega),$$

where

$$B(M,N,\omega) = \frac{4\rho_M}{(\frac{1}{2}M+1)^2\omega^2 - 1} \binom{M+1}{\frac{1}{2}M+1} \left((\tfrac{1}{2}M+1)\omega + \sqrt{(\tfrac{1}{2}M+1)^2\omega^2 - 1} \right)^{-N}, \tag{29}$$

and

$$\rho_M = \begin{cases} (\frac{1}{2}M+1)^2\omega^2 & N \text{ even} \\ (\frac{1}{2}M+1)\omega & N \text{ odd.} \end{cases}$$

Asymptotically, if $M \longrightarrow \infty$ as $N \longrightarrow \infty$, then

$$B(M,N,\omega) = O\left(\frac{2^M}{M^N \omega^N} \right),$$

and if $M \sim N$, then

$$B(M,N,\omega) = O\left(\left(\frac{2}{N\omega} \right)^N \right). \tag{30}$$

Proof. It may be checked that for each x the series (28) is alternating, with the magnitude of the terms decreasing monotonically to zero. One may therefore estimate the series by retaining only its first term, i.e.,

$$\left| f(x) - \frac{p_{N-1}(x)}{q_M(x)} \right| \leq 2 \left| \frac{T_N(x)}{q_M(x)} \right| \left| \frac{q_M((\frac{1}{2}M+1)\omega)}{T_N((\frac{1}{2}M+1)\omega)} \right| \left| \frac{\psi_{\frac{1}{2}M+1}}{x^2 - (\frac{1}{2}M+1)^2\omega^2} \right|.$$

The absolute error is converted to the relative error by dividing both sides by $f(x)$, and then applying the result of Lemma 1, plus the fact that $|\psi_{\frac{1}{2}M+1}| \leq \rho_M$. This yields

$$\left| \frac{f(x) - \frac{p_{N-1}(x)}{q_M(x)}}{f(x)} \right| \leq 2 \binom{M+1}{\frac{1}{2}M+1} \frac{\rho_M}{(\frac{1}{2}M+1)^2\omega^2 - 1} \left| \frac{T_N(x)}{T_N((\frac{1}{2}M+1)\omega)} \right|.$$

The bound (29) is obtained by applying the following inequalities satisfied by the Chebyshev polynomials

$$|T_N(x)| \leq 1, \quad |x| \leq 1; \qquad T_N(x) > \tfrac{1}{2}\left(x + \sqrt{x^2-1} \right)^N, \quad x > 1.$$

To establish the asymptotic behavior of the error bound, one applies Stirling's formula to the result of Lemma 1 to obtain

$$\binom{M+1}{\frac{1}{2}M+1} = O(2^M), \qquad M \longrightarrow \infty.$$

The other factors in (29) are easily estimated. □

Having established the error in the interpolation process, the error in the quadrature process is straightforwardly obtained. Specifically, if $r_{M;N}(x)$ denote the pointwise relative error then

$$f(x) - \frac{p_{N-1}(x)}{q_M(x)} = r_{M;N}(x) f(x).$$

By integrating both sides on $[-1, 1]$ and using the fact that the Rational Fejér Rule integrates the rational function on the left exactly, one obtains

$$\int_{-1}^{1} f(x)\,dx - \sum_{j=1}^{N} w_j f(x_j) = \int_{-1}^{1} r_{M;N}(x) f(x)\,dx.$$

Since $f(x)$ is continuous and positive on $[-1, 1]$ there follows, by Hölder's inequality,

$$\begin{aligned}\left|\int_{-1}^{1} f(x)\,dx - \sum_{j=1}^{N} w_j f(x_j)\right| &\le \int_{-1}^{1} |r_{M;N}(x)| f(x)\,dx \\ &\le \max_{-1\le x\le 1} |r_{M;N}(x)| \int_{-1}^{1} f(x)\,dx,\end{aligned}$$

and hence

$$\left|\frac{\int_{-1}^{1} f(x)\,dx - \sum_{j=1}^{N} w_j f(x_j)}{\int_{-1}^{1} f(x)\,dx}\right| \le \max_{-1\le x\le 1} \left|\frac{f(x) - \frac{p_{N-1}(x)}{q_M(x)}}{f(x)}\right|.$$

The right-hand side has been estimated in the previous theorem. We have therefore proved:

Theorem 6. Let $f(x)$ be defined by (26). Let the poles in the Rational Fejér Rule be defined by (24), for some even integer M. Then the relative error in the N point Rational Fejér Rule, with $N > M$, satisfies

$$\left|\frac{\int_{-1}^{1} f(x)\,dx - \sum_{j=1}^{N} w_j f(x_j)}{\int_{-1}^{1} f(x)\,dx}\right| \le B(M, N, \omega),$$

where $B(M, N, \omega)$ is defined by (29).

In Figure 3 we offer a check on the tightness of the error bound given by Theorem 6. The top two curves represent the theoretical error bound (shown as the dash-dot curve) and the actual error (represented by the dots) in the case when $M = 2$ (fixed). The lower two curves correspond to the choice $M = N - 1$, $N = 3, 5, \ldots$. (As before we used $\omega = 1.001$, $\epsilon = 10^{-14}$.)

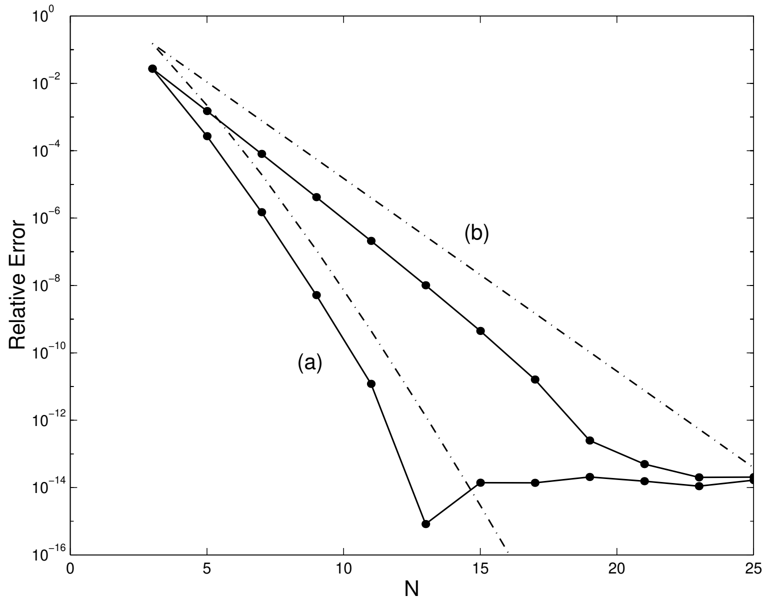

Figure 3. The relative error in the Rational Fejér Rule (black dots), as well as the theoretical error bound (29) (dash-dot curve). The test problem is $I(1.001)$ as defined by (23). In (a) $M = N - 1$, and in (b) $M = 2$ (fixed).

The asymptotic estimate (30) is applicable to the lower pair of curves shown in Figure 3. This estimate confirms an observation that was made in [4] on the basis of numerical evidence, namely that as the singularities approach the interval $[-1, 1]$ (i.e., $\omega \longrightarrow 1$) the convergence rate becomes essentially independent of ω. This is in contrast to polynomial based methods such as Gauss-Legendre or Fejér's first rule, where the convergence rates deteriorate as $\omega \longrightarrow 1$. This is also in contrast to the second test integral (25), in which the accuracy of both the Rational Fejér and Rational Gauss Rules deteriorate as the singularities approach the interval.

The asymptotic convergence rate (30) is of the form $O(r^{-N})$, with $r \longrightarrow 0$ as $N \longrightarrow \infty$. This is the typical rate of convergence of polynomial based quadrature of entire functions. It appears, therefore, that the Rational Fejér Rule has converted the integrand of (23) from a meromorphic function, to effectively an entire function by annihilating the poles nearest $[-1, 1]$ in a systematic manner.

Figure 3 confirms that we have succeeded in our aim of deriving a sharp and computable error bound for the Rational Fejér Rule, at least for the test problem (23). It should be a straightforward matter to generalize the procedure sketched here to produce error estimates also for the integral (25), and indeed any integral where the integrand may be expanded in partial fractions. This will be pursued in a separate study.

6. Conclusions and Future Work

This paper achieved two objectives. First, in Section 3 we introduced new recurrence formulas for computing rational quadrature rules of both interpolatory and Gaussian type. In Section 4 these formulas were shown to be efficient. Second, in Section 2 we extended Fejér's first rule, which is based on polynomial interpolation at the Chebyshev nodes, to the rational case. The numerical results presented in Section 4 have shown that when the cost of constructing the rule is taken into account, the Rational Fejér Rule might be competitive with the rational rules of Gaussian type. An error analysis of the Rational Fejér Rule, as it applies to the test problem (23), was presented in Section 5. The explicitly computable error bounds were shown to be sharp.

Even though we discussed only integrals of constant weight, it should be possible to adapt the algorithms introduced here also to weighted integrals of the form

$$\int_{-1}^{1} w(x) f(x)\, dx.$$

In particular, the algorithms described in Section 3 will remain applicable, provided the integrals (17) and (22) can be computed explicitly when the weight function $w(x)$ is incorporated. It should be noted that the algorithms of [5] do not have such restrictions and are essentially applicable to arbitrary weight functions.

As for future work, the recursive algorithm introduced in Section 3 requires further theoretical investigation; in particular a stability analysis needs to be carried out. We have found experimentally that the algorithm is relatively stable when applied to the test problems (23) and (25) considered here. (This is corroborated to some degree by Figures 2 and 3—note the fact that the error curves remain relatively flat after the relative tolerance 10^{-14} is reached.) For both these examples the poles were distributed symmetrically with respect to the origin. When considering pole distributions that are non-symmetric, such as all $z_j > 1$ for example, the algorithm appears to be unstable. (Of course, since the user is free to choose the poles symmetrically, such an instability may usually be avoided.) Another topic that needs to be addressed is how to modify the algorithm of Section 3 to handle poles of higher multiplicity, as well as how to deal with integrals defined on semi-infinite or infinite intervals.

The Rational Fejér Rule introduced here requires further analysis as well. It would be helpful to be able to tell a priori whether a given choice of poles $\{z_j\}_{j=1}^M$ will lead to positive weights or not. In addition, the convergence proof of Section 5 needs to be generalized. More comprehensive testing needs to be done to decide whether this rule is indeed efficient in comparison with the Rational Gauss Rule, as measured in terms of accuracy achieved per unit of work expended in constructing the rule. These and other issues will be pursued elsewhere.

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