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Linear barycentric rational quadrature

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Abstract Linear interpolation schemes very naturally lead to quadrature rules. Introduced in the eighties, linear barycentric rational interpolation has recently experienced a boost with the presentation of new weights by Floater and Hormann. The corresponding interpolants converge in principle with arbitrary high order of precision. In the present paper we employ them to construct two linear rational quadrature rules. The weights of the first are obtained through the direct numerical integration of the Lagrange fundamental rational functions; the other rule, based on the solution of a simple boundary value problem, yields an approximation of an antiderivative of the integrand. The convergence order in the first case is shown to be one unit larger than that of the interpolation, under some restrictions. We demonstrate the efficiency of both approaches with numerical tests.

1 Introduction: quadrature from equidistant samples

Suppose we are given the discrete data $\mathbf{F} := \{f_0, \ldots, f_n\}$, corresponding to a real or complex function f which is defined and integrable in an interval $[a, b]$ and sampled

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at a strictly ordered set of abscissas $\mathbf{X} := \{x_0 = a, x_1, \ldots, x_{n-1}, x_n = b\}$ in $[a, b]$. Our aim is to either approximate the (definite) integral

$$I := \int_a^b f(x)\,dx \tag{1.1}$$

by a quadrature rule $\sum_{k=0}^n w_k f_k$ or to approximate an antiderivative (primitive) of f.

If we are free to choose the set $\mathbf{X}$ at which the function f is to be sampled, we can opt for any efficient distribution of points. This means using quadrature rules based upon orthogonal polynomials. Examples include Gauss-type rules, which are known to be stable and to converge for every Riemann-integrable function (see for instance [15] or [29]). The situation is different when the set $\mathbf{X}$ cannot be chosen. If the data set stems from measurements, for instance, it is most likely that these are taken on a regular grid. But it is well known that polynomial interpolation from equidistant samples is unstable and that the corresponding Lebesgue constant grows very fast with n (see [24] or [8] and the references therein). As a consequence, Newton–Cotes quadrature rules diverge or are unstable with a growing number of points, as explained in [21, 23] or in [12], where the author shows "die praktische Unbrauchbarkeit dieser Verfahren" (meaning the uselessness of these rules in practice). One way to avoid problems is using composite Newton–Cotes rules of low order such as the composite trapezoidal or Simpson rules. Their frequent use in practical calculations documents the importance of these slowly converging formulas for non-periodic functions, see [13, p. 57] and the included reference to M. Abramowitz. Any attempt to construct geometrically converging interpolants from equidistant data necessarily fails, as it leads to Gibbs and Runge phenomena [22].

In the present paper we shall introduce methods for the approximation of an antiderivative of f by a linear barycentric rational interpolant and of the integral of f by that of such an interpolant. We analyse some of their properties for equidistant points.

2 Linear barycentric rational interpolation

Let us first explicit the linear rational interpolants we shall be using and recall some of their properties.

Let $P_n[f]$ be the unique polynomial of degree at most n interpolating the data $\mathbf{F}$ at the set of nodes $\mathbf{X}$. The steps from the Lagrangian representation to its barycentric form

$$P_n[f](x) = \sum_{k=0}^n \frac{\beta_k}{x - x_k} f_k \Big/ \sum_{k=0}^n \frac{\beta_k}{x - x_k}, \tag{2.1}$$

where the so-called weights β_k are defined by

$$\beta_k = \left[\prod_{j \neq k} (x_k - x_j) \right]^{-1}, \quad k = 0, \ldots, n, \tag{2.2}$$

are explained in many articles, such as [4] and [10]. For details on how to easily implement this interpolant and for explicit $O(n)$ formulas at particular point sets, see [10]. Looking the right way at (2.1) and following [4], we see that $P_n[f]$ interpolates the data $\mathbf{F}$ at the set $\mathbf{X}$, no matter the weights, as long as none of these vanishes. If we replace the weights β_k by other non-zero μ_k, (2.1) usually becomes a true linear rational interpolant

$$r_n[f](x) = \sum_{k=0}^{n} \frac{\mu_k}{x - x_k} f_k \Big/ \sum_{k=0}^{n} \frac{\mu_k}{x - x_k}, \tag{2.3}$$

the numerator and denominator of which are polynomials of degree at most n. By linear we shall mean the linear dependency of $r_n[f]$ on the data $f_0, \ldots, f_n$, this in contrast to the non-linear dependency of the classical rational interpolant, in which the denominator depends on f, see also [6]. Every set of $n+1$ non-zero weights thus defines a new linear rational interpolant. In [4], the second author of the present paper studied the simple choice

$$\overline{\mu}_k = (-1)^k \delta_k, \quad \delta_k := \begin{cases} 1/2, & k = 0 \text{ or } k = n, \\ 1, & \text{otherwise.} \end{cases} \tag{2.4}$$

The corresponding interpolant has no real poles and numerical experiments revealed that the error decreases like $1/n^2$ for large n, see [4]. This choice of weights has been extended by Floater and Hormann in [14]. For every fixed non-negative integer $d \leq n$, the authors considered the set of polynomials $p_i(x)$, $i = 0, \ldots, n - d$, interpolating f at the subsets $\{x_i, \ldots, x_{i+d}\}$ of $\mathbf{X}$ and the rational interpolant

$$r_n[f](x) = \frac{\sum_{i=0}^{n-d} \lambda_i(x) p_i(x)}{\sum_{i=0}^{n-d} \lambda_i(x)}, \tag{2.5}$$

where

$$\lambda_i(x) := \frac{(-1)^i}{(x - x_i) \cdots (x - x_{i+d})}. \tag{2.6}$$

They also found explicit formulas for the interpolation weights μ_k of its barycentric representation. The approximation rate as

$$h := \max_{0 \leq i \leq n-1} (x_{i+1} - x_i) \to 0$$

is $O(h^{d+1})$ for a function $f \in C^{d+2}[a, b]$. One advantage of these interpolants is the fact that the interpolation error depends on the maximum norm of the mere $(d + 2)$-nd order derivative of f, as opposed to the dependence on the $(n + 1)$-st derivative of f in the polynomial case. It turns out that the simple choice (2.4) corresponds to $d = 1$ for equidistant nodes.

3 Integration of barycentric rational interpolants

Every linear interpolation formula

$$f(x) \approx \sum_{k=0}^{n} \gamma_k(x) f_k$$

trivially leads to a linear quadrature rule through the integration of the factors $\gamma_k(x)$. The behaviour of the so-obtained rule regarding convergence and stability simply follows from the respective properties of the interpolant. In the case of an $(n + 1)$-point linear rational interpolant (2.3) with non-zero weights μ_k, we have

$$I = \int_a^b f(x) \, dx \approx \int_a^b r_n[f](x) \, dx$$
$$= \int_a^b \frac{\sum_{k=0}^{n} \frac{\mu_k}{x-x_k} f_k}{\sum_{k=0}^{n} \frac{\mu_k}{x-x_k}} \, dx = \sum_{k=0}^{n} w_k f_k =: Q_n, \qquad (3.1)$$

where

$$w_k := \int_a^b \frac{\frac{\mu_k}{x-x_k}}{\sum_{k=0}^{n} \frac{\mu_k}{x-x_k}} \, dx. \qquad (3.2)$$

If $r_n[f]$ is a true rational interpolant with non-constant denominator, then the so-called quadrature weights w_k can be easily determined in exact arithmetic only if the poles are known.

The choice $\mu_k = \beta_k$ of (2.2) in (3.1) reproduces the Newton–Cotes rules. The same is true if $d = n$ in the interpolant (2.5), since it then coincides with the interpolating polynomial.

For the computation of the weights (3.2), we decided to neglect algebraic methods as they mostly require the polynomials in the numerator and denominator of $r_n[f]$ to be in canonical form. The step from the representation (2.3) of these polynomials to the canonical one is impaired by stability problems [17].

For a rational interpolant whose denominator degree exceeds 4 there is no formula for the poles. As we would like to avoid approximating complex poles and determining expensive partial fraction decompositions, we pursue two ideas for generating linear quadrature rules based on linear rational interpolants.

Under direct rational quadrature we shall here mean the result of applying existing quadrature rules such as Gauss–Legendre or Clenshaw–Curtis [26, 29], which are known to behave well, to approximate the integrals in (3.2).

Indirect rational quadrature uses the fact that the integral (1.1) may be obtained through the solution of an ordinary differential equation, see, e.g., [27, Chap. 12].

4 Direct linear rational quadrature (DRQ)

The linearity of the rational interpolant (2.3) leads to the quadrature rule (3.1) with the weights w_k given by (3.2). Since the integrand in (3.2) is infinitely smooth and

may be evaluated at every point in the interval, we can approximate the integral by any efficient quadrature rule with rapid convergence, such as Gauss–Legendre or Clenshaw–Curtis. Let $w_k^{\mathscr{D}}$, $k = 0, \ldots, n$, be corresponding approximations of the weights in (3.2); the direct rational quadrature rule then replaces Q_n by

$$I = \int_a^b f(x)\, dx \approx \sum_{k=0}^n w_k^{\mathscr{D}} f_k. \tag{4.1}$$

If we do not need the weights, we may apply a rule directly on the whole interpolant, since $r_n[f]$ can be evaluated stably everywhere in the interval. Not evaluating the quadrature weights explicitly can thus make for much faster quadrature. Notice that this could be done as well with the classical non-linear rational interpolant whose barycentric representation is computed in [9].

The convergence of such a quadrature rule is guaranteed, provided the interpolant itself converges. If the interpolation error converges as h^p for some p as $h \to 0$, then the integration error will converge to 0 at least with the same order if we choose a quadrature rule for the integral of $r_n[f]$ that converges at a rate $O(h^q)$ with $q \geq p$; indeed,

$$\left| \int_a^b f(x)\, dx - \sum_{k=0}^n w_k^{\mathscr{D}} f_k \right| \leq \int_a^b |f(x) - r_n[f](x)|\, dx$$

$$+ \left| \int_a^b r_n[f](x)\, dx - \sum_{k=0}^n w_k^{\mathscr{D}} f_k \right|$$

$$\leq C_1 h^p + C_2 h^q \leq C h^p, \tag{4.2}$$

where C, C_1, and C_2 are constants depending only on f, derivatives of f and on the interval length $(b - a)$.

By a similar argument, we see that the degree of precision of the direct rational quadrature rule attains at least the highest integer s such that every polynomial of degree at most s is exactly reproduced by the interpolant.

We have thus established that the integral of every function f with a converging rational interpolant can be approximated, by a direct rational quadrature rule, with at least the same accuracy as the interpolant. For the interpolant (2.5), this yields the following result, which is valid for any distribution of the nodes in **X** and which we shall tighten in some cases (see Sect. 6).

Theorem 4.1 *Suppose n and d, $d \leq n$, are non-negative integers, $f \in C^{d+2}[a, b]$ and $r_n[f]$ is the rational interpolant with parameter d given in (2.5). Let the quadrature weights w_k in (3.2) be approximated by a quadrature rule which converges at least at the rate $O(h^{d+1})$ and has degree of precision at least $d + 1$. Then*

$$\left| \int_a^b f(x)\, dx - \sum_{k=0}^n w_k^{\mathscr{D}} f_k \right| \leq C h^{d+1},$$

where, for $d \geq 1$, C is a constant depending only on d, on derivatives of f and on the interval length. In the case $d = 0$, C is to be multiplied by the mesh ratio

$$\beta = \max_{1 \leq i \leq n-2} \min \left\{ \frac{x_{i+1} - x_i}{x_i - x_{i-1}}, \frac{x_{i+1} - x_i}{x_{i+2} - x_{i+1}} \right\}.$$

The quadrature rule (4.1) *has degree of precision $d + 1$ if $n - d$ is odd and d if $n - d$ is even.*

The ratio β shows up in the corresponding result of [14] as well. The last statement stems from the fact that r_n reproduces polynomials of the said degrees (see Theorem 2 in [14]).

5 Indirect linear rational quadrature (IRQ)

As an alternative to integrating a rational interpolant of f as described in Sect. 4, we shall now follow another approach, in which the integral is seen as the solution of an initial value problem. Approximating I then requires the solution of a full system of linear equations of order n—or an equivalent method—but the procedure yields much more, namely an approximation of an antiderivative of f; I is then automatically approximated by the endpoint value of the latter.

For that purpose, we approximate an antiderivative in the interval $[a, b]$ by a linear rational interpolant

$$r_n[u](x) \approx \int_a^x f(y)\, dy, \tag{5.1}$$

which we determine as the solution of the induced first order initial value problem

$$\frac{d}{dx} r_n[u](x) \approx f(x), \qquad u_0 = r_n[u](a) = 0, \quad x \in [a, b]; \tag{5.2}$$

we solve (5.2) by the collocation solver for boundary value problems introduced in [5] for the second order case.

Here, this merely requires the first derivative at the nodes of a rational interpolant written in barycentric form with non-zero weights. Using Proposition 11 in [25], the authors of [2] established formulas for the computation of such derivatives in matrix form: denote by $\mathbf{u}$ the vector $(u_0, \dots, u_n)^T$ of the unknown values of $r_n[u]$ at the nodes in $\mathbf{X}$ and let $\mathbf{u}'$ be the vector containing the first derivative of $r_n[u]$ at the nodes; then

$$\mathbf{u}' = D\mathbf{u},$$

where the elements of the centro-skew symmetric differentiation matrix D are given by

$$D_{ij} := \begin{cases} \frac{\mu_j}{\mu_i} \frac{1}{x_i - x_j}, & i \neq j, \\ -\sum_{k=0, k \neq i}^{n} D_{ik}, & i = j. \end{cases}$$

As demonstrated in [1], the negative sum should be used for the diagonal elements of such matrices to improve stability. Applying collocation to (5.2) (with the initial condition $u_0 = 0$)—i.e., requiring equality in (5.2) at the nodes $x_1, \ldots, x_n$—leads to a system of n equations for the n unknowns $u_1, \ldots, u_n$:

$$\sum_{j=1}^{n} D_{ij} u_j = f_i, \quad i = 1, \ldots, n. \tag{5.3}$$

Inserting into (2.3) the values u_k obtained from solving this system yields an approximation of an antiderivative of f valid in the whole interval:

$$\int_a^x f(y)\,dy \approx r_n[u](x) = \sum_{k=0}^{n} \frac{\mu_k}{x - x_k} u_k \Big/ \sum_{k=0}^{n} \frac{\mu_k}{x - x_k}, \quad x \in [a, b]. \tag{5.4}$$

At $x = b$, the last expression equals u_n, an approximation of the integral of f over the interval $[a, b]$:

$$\int_a^b f(y)\,dy \approx r_n[u](b) = u_n.$$

We stress that, in contrast with DRQ, IRQ yields not only the value u_n approximating the integral (1.1), but also approximate values of the antiderivative $\int_a^x f(y)\,dy$ at $x_1, \ldots, x_{n-1}$ as $u_1, \ldots, u_{n-1}$ and at all other $x \in [a, b]$ as the interpolant (5.4). For sets of weights μ_k leading to interpolants with no poles in $[a, b]$, this approximate antiderivative is infinitely smooth.

Again, we can derive explicit formulas for the weights of the corresponding quadrature rule. To this end, we use Cramer's rule with the notation of [18], which denotes by $A \underset{n}{\leftarrow} \mathbf{y}$ the matrix A with its nth column replaced by $\mathbf{y}$. Let $\widetilde{D}$ be the differentiation matrix D deprived of its first row and column (recall that $u_0 = 0$), let $\widetilde{\mathbf{f}} := (f_1, \ldots, f_n)^T$ and let $\mathbf{e}_k$ be the kth canonical vector in $\mathbb{R}^n$. Then

$$u_n = \frac{\det(\widetilde{D} \underset{n}{\leftarrow} \widetilde{\mathbf{f}})}{\det(\widetilde{D})} = \sum_{k=1}^{n} w_k^{\mathscr{I}} f_k,$$

where the quadrature weights are given by

$$w_k^{\mathscr{I}} := \frac{\det(\widetilde{D} \underset{n}{\leftarrow} \mathbf{e}_k)}{\det(\widetilde{D})}, \quad k = 1, \ldots, n.$$

6 Properties of DRQ in the case of equidistant nodes

In this section we study the theoretical behaviour of DRQ when the rational interpolant $r_n[f]$ in (3.1) is a member of the family of linear rational interpolants (2.5). It is important to remember that these rational interpolants are infinitely smooth (even analytic) and have no real poles (see Theorem 1 in [14]). Moreover, the Lebesgue constant associated with equidistant nodes increases only logarithmically with n for

fixed d, see [11]. We shall first investigate the convergence rates of the DRQ rules for equidistant nodes. We show that, in this special case, the rate of approximation of the quadrature rule is $O(h^{d+2})$ when the rational interpolant converges at the rate $O(h^{d+1})$. At the end of this section we establish the degree of precision and the symmetry of these rules. Some of the tools we use in the proofs stem from [20].

Let us begin with a symmetry property of the denominator of the rational interpolant (2.5). In what follows, we denote this denominator by

$$\Lambda_n(x) := \sum_{i=0}^{n-d} \lambda_i(x) \tag{6.1}$$

and call $\overline{x} := \frac{a+b}{2}$ the midpoint of the interval $[a, b]$.

Lemma 6.1 *Suppose the nodes x_i, $i = 0, \ldots, n$, are distributed symmetrically about $\overline{x}$, i.e., $(\overline{x} - x_i) = (x_{n-i} - \overline{x})$ for all i. Then the denominator in (2.5) is either symmetric or anti-symmetric about $\overline{x}$, in the sense that for every real x,*

$$\Lambda_n(\overline{x} + x) = (-1)^{n+1} \Lambda_n(\overline{x} - x). \tag{6.2}$$

Proof We show that for every $i \in \{0, \ldots, n - d\}$ the following identity holds:

$$\lambda_i(\overline{x} + x) = (-1)^{n+1} \lambda_{n-d-i}(\overline{x} - x). \tag{6.3}$$

By the definition (2.6), we have

$$\lambda_i^{-1}(\overline{x} + x) = (-1)^i \prod_{k=0}^{d} (\overline{x} + x - x_{i+k}).$$

Since the nodes are distributed symmetrically about $\overline{x}$, it follows that the above right hand side equals

$$(-1)^{i+d+1} \prod_{k=0}^{d} (\overline{x} - x - x_{n-i-k}).$$

Inverting the order of the factors in the last product, we obtain (6.3). □

For the next steps, we use the real functions

$$\Omega_n(y) := \int_{x_{d+1}}^{y} \frac{1}{\Lambda_n(x)} \, dx. \tag{6.4}$$

This definition trivially leads to the following corollary of Lemma 6.1.

Corollary 6.1 *For any positive integers n and d, $d \leq n$,*

$$
\begin{aligned}
&\Omega_n(x_{d+1}) = 0, \\
&\Omega_n(x_{n-d-1}) = 0, && \text{if } n \text{ is even,} \\
&\Omega_n(x_{n-d-1}) = 2\Omega_n(\overline{x}), && \text{if } n \text{ is odd.}
\end{aligned}
$$

Before we state the next lemma, we recall from [14] that the reciprocal of the denominator $\Lambda_n(x)$ may be rewritten as

$$\frac{1}{\Lambda_n(x)} = (-1)^{n-d} \frac{L(x)}{s(x)}, \quad \text{where } L(x) = \prod_{i=0}^{n} (x - x_i) \tag{6.5}$$

and where $s(x)$ is positive for all real x, as shown in Theorem 1 of the same article. This means that the reciprocal of the denominator changes sign only at the $n + 1$ nodes x_i.

The following lemma will be essential for our proof of the convergence rates.

Lemma 6.2 *Suppose the nodes* x_i, $i = 0, \ldots, n$, *are equidistant. Then* Ω_n *does not change sign in* (x_{d+1}, x_{n-d-1}). *In particular, if* $d \le n/2 - 1$, *then*

$$\Omega_n(y) < 0. \tag{6.6}$$

Proof We will show (6.6) only for $d \le n/2 - 1$ and $y \in (x_{d+1}, \overline{x})$. The other cases then become obvious from Lemma 6.1. The claim (6.6) remains to be checked at $y = x_{d+3}, x_{d+5}, \ldots$ in $(x_{d+1}, \overline{x})$, since by (6.5) the function $1/\Lambda_n(x)$ changes sign exclusively at the nodes x_i and is negative in (x_{d+1}, x_{d+2}), independently of n and d. In order to prove (6.6), we show that

$$\int_{x_k}^{x_{k+2}} \frac{1}{\Lambda_n(x)} \, dx < 0, \tag{6.7}$$

for $k = d + 1, d + 3, \ldots$ such that $[k, k + 2] \subseteq [d + 1, n/2]$. This means that every negative contribution to $\Omega_n(y)$ dominates the positive contribution that immediately follows it. It is then easy to see that the remaining contribution to $\Omega_n(n/2)$ is also negative, if it occurs.

We first transform (6.7) into an integral over one sub-interval

$$\int_{x_k}^{x_{k+2}} \frac{1}{\Lambda_n(x)} \, dx = \int_{x_k}^{x_{k+1}} \left(\frac{1}{\Lambda_n(x)} + \frac{1}{\Lambda_n(x + h)} \right) dx.$$

Since the nodes are equidistant, we can express $\Lambda_n(x + h)$ in terms of $\Lambda_n(x)$:

$$\Lambda_n(x + h) = \lambda_0(x + h) - \Lambda_n(x) + \lambda_{n-d}(x). \tag{6.8}$$

This lets us further modify (6.7) into

$$\int_{x_k}^{x_{k+2}} \frac{1}{\Lambda_n(x)} \, dx = \int_{x_k}^{x_{k+1}} \frac{\lambda_0(x + h) + \lambda_{n-d}(x)}{\Lambda_n(x)\Lambda_n(x + h)} \, dx.$$

Finally, we discuss the sign of the last integrand. The denominator is negative since $x \in (x_k, x_{k+1})$ and $\Lambda_n(x)$ changes sign at the nodes. As $x \ge x_{d+1}$, we see from (2.6) that $\lambda_0(x + h)$ is positive. Moreover, $\lambda_{n-d}(x)$ is smaller in magnitude than $\lambda_0(x + h)$ for $x \le \overline{x}$. Thus the numerator is positive and the left hand side of (6.6) may be interpreted as a sum of negative terms. $\qquad\square$

An essential ingredient of our proof of the convergence rates will be the following change of variable:

$$x = a + th, \quad t \in [0, n]. \tag{6.9}$$

It will enable us to separate the powers of h from the constant factor in the error term. As a preparation, we introduce the functions

$$\overline{\lambda}_i(t) := \frac{(-1)^i}{(t - i) \cdots (t - (i + d))}, \quad i = 0, \ldots, n - d, \quad \text{and} \quad \overline{\Lambda}_n(t) := \sum_{i=0}^{n-d} \overline{\lambda}_i(t),$$

which are the $\lambda_i(x)$ defined in (2.6), respectively $\Lambda_n(x)$ from (6.1), after changing the variable and neglecting the powers of h.

The next lemma shows that the integral of $\overline{\lambda}_0$ is bounded.

Lemma 6.3 *For any positive integers n and d, $d \leq n$, the integral*

$$\int_{d+1}^{n/2} \overline{\lambda}_0(t + 1) \, dt$$

is bounded as a function of n.

Proof We first observe that, after a partial fraction decomposition, $\overline{\lambda}_0(t + 1)$ may be expressed as

$$\overline{\lambda}_0(t + 1) = \sum_{i=0}^{d} \frac{C_i}{t + 1 - i}, \quad \text{where} \quad C_i := \frac{(-1)^{i+d}}{i!(d - i)!}.$$

This expression is now easy to integrate,

$$\int_{d+1}^{n/2} \overline{\lambda}_0(t + 1) \, dt = \sum_{i=0}^{d} C_i \ln\left(\frac{n}{2} + 1 - i\right) - \sum_{i=0}^{d} C_i \ln(d + 2 - i).$$

As the last term does not depend on n, it is constant for fixed d. We will show that the first converges towards 0 as $n \to \infty$ for fixed d. To this end, we use the property of the ln function to transform products into sums,

$$\sum_{i=0}^{d} C_i \ln\left(\frac{n}{2} + 1 - i\right) = \frac{(-1)^d}{d!} \sum_{i=0}^{d} (-1)^i \binom{d}{i} \ln\left(\frac{n}{2} + 1 - i\right)$$

$$= \frac{(-1)^d}{d!} \ln\left(\frac{P(n/2)}{Q(n/2)}\right),$$

where P and Q are monic polynomials of the same degree in $n/2$, since $\sum_{i=0}^{d}(-1)^i \binom{d}{i} = 0$. Consequently, this term vanishes as $n \to \infty$. $\qquad \square$

As a last preparation for the main results, we prove yet another lemma.

Lemma 6.4 *For any positive integers n and d, d ≤ n/2 − 1, the expressions*

$$\int_{d+1}^{n/2} \frac{1}{\overline{\Lambda}_n(t)}\, dt \quad and \quad \int_{d+1}^{n/2} \frac{(t-n/2)/n}{\overline{\Lambda}_n(t)}\, dt$$

are bounded as functions of n.

Proof As in the proof of Lemma 6.2, we may split the integrals into two parts. To this end, we define the set

$$\mathcal{K} := \left\{ k = d+1, d+3, \dots \,\middle|\, [k, k+2] \subset \left[d+1, \frac{n}{2} \right] \right\}.$$

Moreover let

$$\mathcal{R} := [d+1, n/2] \setminus \bigcup_{k \in \mathcal{K}} [k, k+2]$$

be the remaining part of the interval $[d + 1, n/2]$. Now the integrals over $\mathcal{R}$ are clearly bounded, since $\overline{\Lambda}_n(t)$ is bounded from below as shown in Theorems 2 and 3 from [14] and $(t − n/2)/n$ is smaller than $1/2$ in norm for $0 \le t \le n/2$. We proceed to show the boundedness of the first part of the first integral,

$$\sum_{k \in \mathcal{K}} \int_k^{k+2} \frac{1}{\overline{\Lambda}_n(t)}\, dt = \sum_{k \in \mathcal{K}} \int_k^{k+1} \frac{\overline{\lambda}_0(t+1) + \overline{\lambda}_{n-d}(t)}{\overline{\Lambda}_n(t)\overline{\Lambda}_n(t+1)}\, dt.$$

We have shown in the proof of Lemma 6.2 that the integrand does not change sign. Thus we may study the denominator separately. Its reciprocal is bounded by C^2, where $C = d!$ if $d \ne 0$ and $C = 2$ if $d = 0$. Thus we may write

$$\left| \sum_{k \in \mathcal{K}} \int_k^{k+2} \frac{1}{\overline{\Lambda}_n(t)}\, dt \right| \le C^2 \left| \int_{d+1}^{n/2} \overline{\lambda}_0(t+1)\, dt + \int_{d+1}^{n/2} \overline{\lambda}_{n-d}(t)\, dt \right|.$$

The first term is covered by Lemma 6.3 and the second is obviously bounded by $(n/2)\overline{\lambda}_{n-d}(n/2)$, which converges towards a constant for $d = 0$ and vanishes as $n \to \infty$ if $d > 0$.

To deal with the second integral of the claim, we proceed analogously. First, we observe that

$$\sum_{k \in \mathcal{K}} \int_k^{k+2} \frac{(t-n/2)/n}{\overline{\Lambda}_n(t)}\, dt$$

$$= \sum_{k \in \mathcal{K}} \frac{1}{n} \int_k^{k+1} \frac{(t - n/2)(\overline{\lambda}_0(t+1) + \overline{\lambda}_{n-d}(t)) + \overline{\Lambda}_n(t)}{\overline{\Lambda}_n(t)\overline{\Lambda}_n(t+1)}\, dt.$$

Similar arguments as above lead to

$$\left| \sum_{k \in \mathcal{K}} \int_k^{k+2} \frac{(t-n/2)/n}{\overline{\Lambda}_n(t)}\, dt \right| \le \frac{C^2}{2} \left| \int_{d+1}^{n/2} \overline{\lambda}_0(t+1)\, dt + \frac{n}{2}\overline{\lambda}_{n-d}(n/2) \right| + \frac{C}{2},$$

which is clearly bounded. □

The preceding lemmas help us to prove the main results.

Theorem 6.1 *Suppose n and d, $d \leq n/2 - 1$, are non-negative integers, $f \in C^{d+3}[a, b]$ and $r_n[f]$ is the rational interpolant with parameter d given in (2.5) and interpolating f at equidistant nodes. Let the quadrature weights w_k in (3.2) be approximated by a quadrature rule converging at least at the rate $O(h^{d+2})$. Then*

$$\left| \int_a^b f(x)\, dx - \sum_{k=0}^n w_k^{\mathscr{Q}} f_k \right| \leq Ch^{d+2},$$

where C is a constant depending only on d, on derivatives of f and on the interval length $b - a$.

The hypothesis $d \leq n/2 - 1$ is no real limitation for two reasons. Firstly, d is meant to be fixed in advance and not to depend on n. In consequence the hypothesis on d will become fulfilled as n increases. Secondly, if $d \geq n/2$, we can use Theorem 4.1 and (4.2) to change the factor $b - a$ into $2dh$ and derive an error bound depending on h^{d+2}.

Proof As exemplified in (4.2) it is sufficient to study the integral of the interpolation error,

$$\int_a^b \left(f(x) - r_n[f](x) \right) dx. \tag{6.10}$$

Following [14], we rewrite the interpolation error at $x \in [a, b]$ as

$$f(x) - r_n[f](x) = \frac{\sum_{i=0}^{n-d} (-1)^i f[x_i, \ldots, x_{i+d}, x]}{\sum_{i=0}^{n-d} \lambda_i(x)} =: \frac{F_n(x)}{\Lambda_n(x)}.$$

The authors show in the same article that the numerator F_n is bounded by a constant depending only on d, on low order derivatives of f and on the interval length. In what follows, such bounds will be denoted generically by C.

Our study of (6.10) begins with a splitting of the integral into three parts

$$\int_a^b \left(f(x) - r_n[f](x) \right) dx = \int_a^{x_{d+1}} \frac{F_n(x)}{\Lambda_n(x)}\, dx + \int_{x_{d+1}}^{x_{n-d-1}} \frac{F_n(x)}{\Lambda_n(x)}\, dx$$

$$+ \int_{x_{n-d-1}}^b \frac{F_n(x)}{\Lambda_n(x)}\, dx.$$

The first and last parts are bounded by Ch^{d+2}: simply apply the change of variable (6.9) and take the maximum norm. The difficult part is the second one. We will show that the oscillations of the reciprocal of $\Lambda_n(x)$ almost cancel throughout that central part of the interval $[a, b]$. To see this, we recall the definition (6.4) of Ω_n and integrate by parts:

$$\int_{x_{d+1}}^{x_{n-d-1}} \frac{F_n(x)}{\Lambda_n(x)}\, dx = F_n(x_{n-d-1})\Omega_n(x_{n-d-1}) - \int_{x_{d+1}}^{x_{n-d-1}} F_n'(x)\Omega_n(x)\, dx.$$

On account of Corollary 6.1 we know that $\Omega_n(x_{n-d-1})$ vanishes if n is even. If n is odd, it equals $2\Omega_n(\overline{x})$, which with the change of variable (6.9) and by Lemma 6.4 may be bounded by Ch^{d+2}. Lemma 6.2 enables us to deal with the second term by applying the mean value theorem for integrals:

$$\int_{x_{d+1}}^{x_{n-d-1}} F_n'(x)\Omega_n(x)\,dx = F_n'(\xi) \int_{x_{d+1}}^{x_{n-d-1}} \Omega_n(x)\,dx$$

for some $\xi \in [x_{d+1}, x_{n-d-1}]$. Since we assume that $f \in C^{d+3}[a,b]$, $F_n'(\xi)$ is bounded by a constant, as shown in [7] (see also [20]). As $x - \overline{x}$ is an antiderivative of 1, one more integration by parts yields

$$\int_{x_{d+1}}^{x_{n-d-1}} \Omega_n(x)\,dx = (x_{n-d-1} - \overline{x})\Omega_n(x_{n-d-1}) - \int_{x_{d+1}}^{x_{n-d-1}} \frac{x - \overline{x}}{\Lambda_n(x)}\,dx.$$

If n is odd, the last integral vanishes as its integrand is anti-symmetric about $\overline{x}$ by a trivial modification of Lemma 6.1. If n is even, we repeat the change of variable (6.9) and we use the symmetry of the integrand about $\overline{x}$. To conclude by means of Lemma 6.4, we recall that $h = (b-a)/n$. $\qquad\square$

Lemma 6.1 and Corollary 6.1 of this section enable us to show a more general result about the degree of precision (as defined, e.g., in [20]) of the DRQ rule with a rational interpolant (2.5) from [14]. The nodes only need to be distributed symmetrically about $\overline{x}$.

Theorem 6.2 *Suppose n and d, $d \leq n$, are non-negative integers, r_n in the DRQ rule is the rational interpolant with parameter d given in (2.5) and the nodes x_i are distributed symmetrically about $\overline{x}$. Let the linear quadrature rule Q approximating the integral of r_n be symmetric and have degree of precision at least $d+2$. Then the resulting DRQ rule has degree of precision*

$$\begin{array}{ll} d+2, & \textit{if } n \textit{ is even and } d \textit{ is odd}, \\ d+1, & \textit{if } n \textit{ and } d \textit{ are even}, \\ d+1, & \textit{if } n \textit{ is odd and } d \textit{ is even}, \\ d, & \textit{if } n \textit{ and } d \textit{ are odd}. \end{array}$$

Proof The last two claims follow immediately from Theorem 2 in [14], since r_n exactly reproduces polynomials of degree $d+1$, respectively d, in these cases.

The proof for the remaining claims will be divided into two parts. Firstly, we show that the interpolation error for x^{d+2}, respectively x^{d+1}, is anti-symmetric about $\overline{x}$. Secondly, we use this result to prove that x^{d+2}, respectively x^{d+1}, are integrated exactly by DRQ in these cases.

We begin with the case where n is even and d is odd. Following the lines of the proof of Theorem 2 in [14] for $f(x) = x^{d+2}$, we write the interpolation error for $x \in [a,b]$ as

$$r_n[x^{d+2}](x) - x^{d+2} = \sum_{i=0,\ i \text{ even}}^{n-d-1} (x_{i+d+1} - x_i)x^{d+2}[x_i, \ldots, x_{i+d+1}, x]\bigg/ \Lambda_n(x),$$

where $x^{d+2}[x_i, \ldots, x_{i+d+1}, x]$ stands for the corresponding divided difference of order $d + 3$ of x^{d+2}, which equals 1 (see for example [20]). Thus the numerator is constant and the whole function is anti-symmetric by Lemma 6.1. Similar arguments may be used for the case where both n and d are even.

Now we treat the second part of the proof. To this aim let $P(x)$ be the polynomial under consideration, that is, either x^{d+2} or x^{d+1}. As the linear quadrature rule Q has degree of precision at least $d + 2$, the total quadrature error of the DRQ rule is

$$\int_a^b P(x)dx - Q[r_n[P]] = \left(\int_a^b P(x)dx - Q[P] \right) + \left(Q[P] - Q[r_n[P]] \right)$$

$$= Q[P - r_n[P]].$$

Since Q is assumed to be symmetric and the interpolation error $P(x) - r_n[P](x)$ is anti-symmetric, this quadrature error vanishes. $\qquad\square$

Finally we use Lemma 6.1 to show that the DRQ rule with a rational interpolant (2.5) from [14] is symmetric if the nodes are distributed symmetrically about $\overline{x}$.

Theorem 6.3 *The DRQ rule* (4.1) *as determined by the hypotheses of the previous theorem is symmetric.*

Proof We show that the Lagrange fundamental rational functions

$$R_k(x) := \frac{\mu_k}{x - x_k} \Big/ \Lambda_n(x)$$

are pairwise symmetric about $\overline{x}$, that is

$$R_k(\overline{x} + x) = R_{n-k}(\overline{x} - x)$$

for every real x. The symmetry of Q then guarantees that $w_k^{\mathscr{D}} = w_{n-k}^{\mathscr{D}}$. Note that the denominator in the barycentric representation (2.3) of r_n equals the denominator in (2.5), see [14]. The denominator $\Lambda_n(x)$ does not depend on k and we know from Lemma 6.1 that (6.2) holds. As the nodes are supposed to lie symmetrically about $\overline{x}$, we see that $\overline{x} + x - x_k = -(\overline{x} - x - x_{n-k})$. We finally show that

$$\mu_k = (-1)^n \mu_{n-k}. \qquad (6.11)$$

The barycentric weights are given in [14] as

$$\mu_k = (-1)^{k-d} \sum_{i \in J_k} \prod_{j=i, \, j \neq k}^{i+d} |x_k - x_j|^{-1}, \qquad (6.12)$$

where

$$J_k = \{i \in \{0, \ldots, n - d\} | k - d \leq i \leq k\}.$$

Table 1 Error with the direct and indirect rational quadrature rules

n	Runge ($d = 3$)				Sine ($d = 4$)			
	DRQ	Order	IRQ	Order	DRQ	Order	IRQ	Order
10	7.5e−02		4.0e−01		2.5e−03		1.1e−01	
20	1.3e−03	5.8	1.0e−02	5.3	5.0e−05	5.6	5.0e−03	4.4
40	1.0e−06	10.3	4.6e−05	7.8	7.8e−07	6.0	1.9e−04	4.7
80	6.0e−09	7.4	4.9e−06	3.2	1.2e−08	6.0	7.6e−06	4.7
160	1.8e−10	5.1	4.2e−07	3.6	1.8e−10	6.0	3.1e−07	4.6
320	5.4e−12	5.0	3.6e−08	3.5	2.9e−12	6.0	1.3e−08	4.6
640	2.1e−13	4.7	3.2e−09	3.5	9.0e−14	5.0	5.8e−10	4.5

The fact that, by the symmetry of the nodes,

$$|x_k - x_j| = |x_{n-k} - x_{n-j}|$$

and a rearrangement of the factors in the product and of the terms in the sum in (6.12) yield (6.11). □

7 Numerical results

To illustrate the theoretical results from Sect. 6 and the efficiency of the methods introduced in this paper, we have approximated the integral and the antiderivative of two functions, Runge's $f_1(x) = 1/(1 + x^2)$ and $f_2(x) = \sin(x)$. We sampled them both at *equidistant nodes*, f_1 in the interval $[-5, 5]$. We investigated f_2 in the non-symmetric interval $[-4, 5]$ to avoid an approximation of 0, since the DRQ rule is symmetric and f_2 is anti-symmetric. We used the rational interpolant (2.5) with the same d as in [14], i.e., $d = 3$ for f_1 and $d = 4$ for f_2.

Our aim was to observe estimated approximation orders with the DRQ and IRQ rules. We computed the DRQ rule by the Gauss–Legendre rule with 1000 points. This may seem expensive at first sight. However the Chebfun [3, 28] command legpts, an implementation of the method introduced in [16], provides a very fast algorithm. Moreover, we had to compute the Legendre points and weights only once for all the examples we investigated. For the antiderivative, we considered the error at 2000 equidistant points in the interval $[5a/4, 5b/4]$, computed the maximum value inside the interval $[a, b]$ and deduced the convergence rates.

Table 1 illustrates Theorem 6.1 on the convergence rates of the DRQ rule. We find experimental orders of about 5 for the approximation of the integral of f_1 and 6 for that of f_2 for large enough n, in accordance with the predicted $d + 2$. With the IRQ rule, the order is smaller than with DRQ. Several examples, including those displayed here, show an experimental order of $d + 1/2$.

We do not explicit the results on the approximation of antiderivatives of f_1 and f_2 since they are very similar to the results obtained with IRQ, which is to be expected from its definition. Figure 1 reveals the quality of the approximation of an antiderivative with our indirect rational method with $d = 3$ and $n = 9$. The solid line

Fig. 1 Approximating an antiderivative of Runge's example with $d = 3$ and $n = 9$
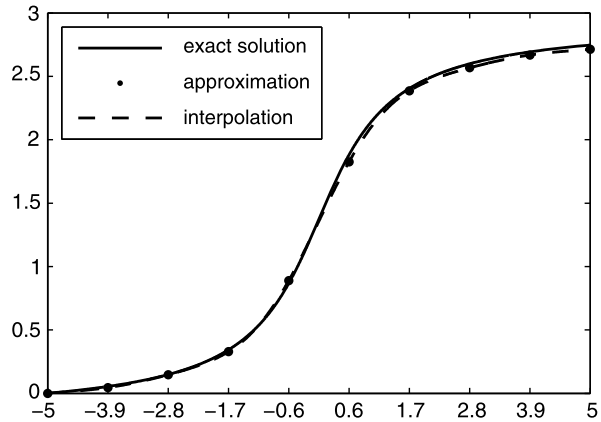

represents the solution of the problem $u' = f_1$, $u(0) = 0$, the dots are the approximations $u_0, \ldots, u_9$ and the dashed line is the corresponding rational interpolant.

The slower convergence of the IRQ rule as compared with the DRQ rule is one reason why we did not study further the theoretical convergence behaviour of the former. Additionally, we observed that some of the quadrature weights in the IRQ rule are negative for almost every admissible choice of n and d. On the other hand, numerical tests revealed that the weights in the DRQ rule, computed using the 1000-point Gauss–Legendre rule, are positive at least for n between d and 1250 for $0 \leq d \leq 5$. In consequence, these rules are stable and converge for every Riemann-integrable function, see [12] and [19].

In a second experiment, we have compared graphically the DRQ and IRQ rules for various rather low values of d, namely $d = 5, 6, 7$, with Newton–Cotes rules, see Fig. 2. We sampled the function $\sin(100x) + 100$ at equidistant nodes and repeated the same computations as in the previous examples. The standard Newton–Cotes rules (for $d = n$) are known to be unstable and to diverge with a growing number of points. We omit to plot their catastrophic behaviour here and concentrate on the composite Simpson rule and on the composite Boole rule (Newton–Cotes with 5 points). The slopes of the curves reflect the experimental order 4 of the composite Simpson rule for sufficiently large n [13] and the order 6 of the composite Boole rule. We see here, in the top picture for DRQ and in the bottom one for IRQ, rapidly decreasing errors for our quadrature rules based on linear barycentric rational interpolants interpolating between a large number of equidistant points. With an adequate choice of the parameter d, these quadrature rules outperform composite Newton–Cotes rules, including those with higher theoretical convergence rates; we do not show the corresponding results. For small to moderate values of n, the error of composite Simpson is smallest in this example: for such n, the piecewise parabolic interpolant turns out to be more accurate than the (infinitely smooth) linear rational one. Notice that in our rules n may be any positive number, whereas it must be of the form $2k + 1$ in composite Simpson and $4k + 1$ in composite Boole.

Finally we have repeated the experiments of the present section using spline interpolants of degree d with the not-a-knot end condition, computed with MATLAB's

Fig. 2 Comparison of the errors in the composite Simpson and Boole rules with DRQ (*top*) and with IRQ (*bottom*) for $16 \leq n \leq 1024$
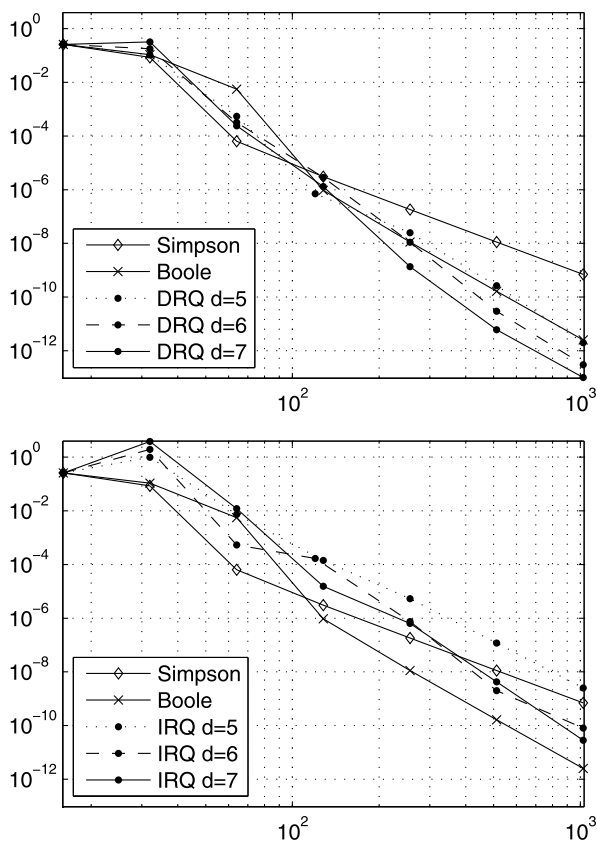
spline toolbox. We omit to present the results since these spline-based methods yield almost identical errors as the DRQ rules in our examples.

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