

Recent advances in linear barycentric rational interpolation[☆]

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Well-conditioned, stable and infinitely smooth interpolation in arbitrary nodes is by no means a trivial task, even in the univariate setting considered here; already the most important case, equispaced points, is not obvious. Certain approaches have nevertheless experienced significant developments in the last decades. In this paper we review one of them, linear barycentric rational interpolation, as well as some of its applications.

1. Introduction

The infinitely smooth interpolation of smooth functions between equispaced or arbitrarily spaced points on a finite interval is a very natural problem. It is not an easy one, though. Many approaches, such as the simplest, the interpolating polynomial, are unstable or even ill-conditioned: several suffer from Runge's phenomenon, i.e., the interpolant of many functions diverges in the vicinity of the interval's boundary. Among the most efficient methods are Fourier continuation and radial basis functions; an extensive review is being prepared by R. Platte.

In 2005, the first author, together with R. Baltensperger and H. Mittelmann, published an overview on barycentric rational interpolation [1] which classified rational methods in two classes: on one hand the (classical) *nonlinear* ones, in which, among other features, the denominator of the interpolant is allowed to depend on the interpolated function f , and on the other hand the *linear* ones, in which the denominator depends on the nodes but not on f ; in the latter case, as the name tells, the interpolant is linear in f , which is necessary, e.g., in cases when one wishes to use it as an ansatz for the solution of equations.

The linear methods presented by the first author in [2] are extremely stable, but converge too slowly for arbitrary interpolation nodes and, unfortunately, for the most important case of equispaced nodes. However, when one may choose the nodes, the second linear rational interpolant introduced in [2], when combined with nodes which are conformal maps of Chebyshev points, provides a very efficient means (in the sense that it is as simple as the polynomial interpolant and exponential convergence occurs) of solving various kinds of differential equations with steep solutions [3–6].

Shortly after the publication of [1], the paper [7] dramatically changed the situation by giving linear rational interpolants which, in principle, converge with an arbitrary high order for most sets of interpolation points, in particular equispaced

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ones. Despite its short existence, this paper has already led to several extensions and applications, some of which we intend to summarize in the present paper.

In Section 2, we review the steps leading from polynomial to rational interpolation in their barycentric forms; in Section 3, we present the linear case addressed in this work. Section 4 describes the example of the Floater and Hormann family of linear rational interpolants, while Section 5 summarizes the extension by the second author of the present article. Then applications are described: approximation of derivatives in Sections 6 and 7, rational finite differences in Section 8, quadrature and approximation of antiderivatives in Section 9.

2. From polynomial to rational interpolation

In this section we review some facts about polynomial and rational interpolation in barycentric form, concentrating on the linear case. Let $n + 1$ distinct points (or *nodes*) $x_0, x_1, \dots, x_n, a \leq x_j \leq b$, and $f_j := f(x_j)$ corresponding values of a function f be given. Then there exists a unique polynomial $p_n[f]$ of degree at most n which interpolates f , i.e., satisfies $p_n[f](x_j) = f_j, j = 0, 1, \dots, n$. Its *Lagrange form* is given by

$$p_n[f](x) := \sum_{j=0}^n f_j \ell_j(x), \quad \ell_j(x) := \prod_{k \neq j} \frac{(x - x_k)}{(x_j - x_k)}. \quad (2.1)$$

The leading factors of the ℓ_j ,

$$v_j := \prod_{k \neq j} \frac{1}{x_j - x_k}, \quad j = 0, 1, \dots, n,$$

which in the context of barycentric interpolation are called *weights* and do not depend on f , may be computed beforehand. (Note that there have recently been some advances in this calculation [8].) Setting

$$\ell(x) := \prod_{k=0}^n (x - x_k),$$

one may rewrite the polynomial in its *first barycentric form*

$$p_n[f](x) = \ell(x) \sum_{j=0}^n \frac{v_j}{x - x_j} f_j,$$

which enjoys several advantages over Lagrange's formula (2.1), among them

- evaluation in $\mathcal{O}(n)$ operations, once the v_j have been computed;
- ease of adding new data (x_{n+1}, f_{n+1}) and, above all,
- backward stability of the evaluation of $p_n[f]$ [9].

A classical result says that the interpolating polynomial is very ill-conditioned for equispaced nodes. With *linear* interpolation operators \mathcal{L} , the condition is measured by the *Lebesgue constant*, i.e., the norm

$$\sup_{f \in \mathcal{C} \setminus \{0\}} \frac{\|\mathcal{L}f\|}{\|f\|}$$

of the linear operator which to every f associates its interpolant. (In this work $\|\cdot\|$ denotes the maximum norm.)

When the interpolation operator may be written in Lagrange form

$$\mathcal{L}f(x) = \sum_{j=0}^n f_j L_j(x), \quad L_j(x_i) = \delta_{ij},$$

the Lebesgue constant, often denoted by Λ_n , turns out to be the maximum of the *Lebesgue function* [10]

$$\Lambda(x) := \sum_{j=0}^n |L_j(x)|.$$

For p_n ($L_j := \ell_j$) and equispaced points, one has $\Lambda_n \sim \frac{2^{n+1}}{en \ln n}$ [11], and Λ shows much larger local maxima near the extremities than in the middle of the interval. Fig. 1 displays the Lebesgue function associated with polynomial interpolation in 11 equispaced nodes.

The unicity implies that the constant function $f \equiv 1$ is represented exactly by its polynomial interpolant:

$$p_n[1](x) = \ell(x) \sum_{j=0}^n \frac{v_j}{x - x_j} = 1.$$

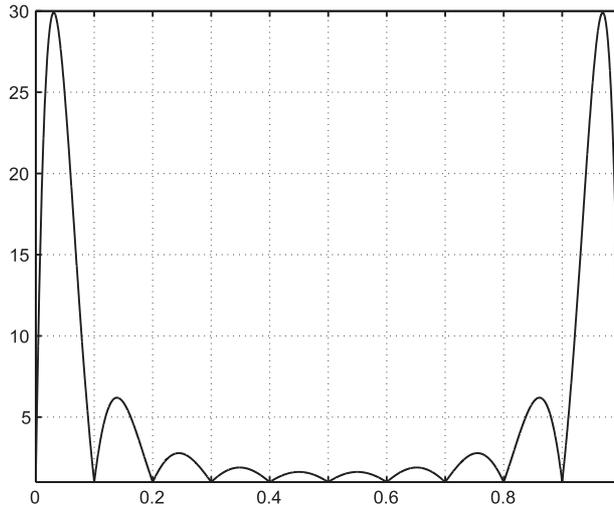


Fig. 1. Lebesgue function associated with polynomial interpolation in 11 equispaced nodes.

Dividing $p_n[f]$ by $p_n[1]$ and canceling ℓ gives the (true) barycentric form of the polynomial interpolant,

$$p_n[f](x) = \frac{\sum_{j=0}^n \frac{v_j}{x - x_j} f_j}{\sum_{j=0}^n \frac{v_j}{x - x_j}}. \quad (2.2)$$

This formula has some advantages: besides the fact that ℓ does not appear any longer, the quotient leads to a cancellation of common factors and thus to *simplified weights*, which diminish the risk of overflow: for equispaced nodes,

$$v_j^* = (-1)^j \binom{n}{j};$$

such closed formulas also exist for Chebyshev nodes [12] and in a certain sense for Gauss–Legendre nodes [13].

Moreover, the interpolation property is extremely stable with respect to the weights: as noticed in [14], with (2.2),

$$\lim_{x \rightarrow x_\ell} \frac{\sum_{j=0}^n \frac{v_j}{x - x_j} f_j}{\sum_{j=0}^n \frac{v_j}{x - x_j}} = f_\ell \quad \forall v_\ell \neq 0. \quad (2.3)$$

Multiplying back by ℓ shows that (2.3) now generically is a *rational* interpolant of f . Conversely, the following lemma guarantees that every rational interpolant may be written in barycentric form.

Lemma 2.1 ([15]). *Let $\{x_j\}$, $j = 0, 1, \dots, n$, be $n + 1$ distinct nodes, $\{f_j\}$ corresponding real numbers. Then every rational interpolant of the f_j with numerator and denominator degrees both at most n may be written in barycentric form, for some weights v_j .*

3. Linear rational interpolation

In the barycentric form (2.2) of the polynomial interpolant, the weights v_j are chosen in such a way that

$$\ell(x) \sum_{j=0}^n \frac{v_j}{x - x_j} = 1.$$

The idea behind linear rational interpolation, as introduced in [2], is to choose (through its weights v_j) for any given set of nodes a *denominator that depends on the nodes* but still not on the function, so as to maintain the linearity of the interpolation. Following [16], we will denote the resulting interpolant by $r_n[f]$. It requires the nodes to be strictly ordered, i.e., $x_0 < x_1 < x_2 < \dots < x_n$.

When the numerator does not have common factors $x - x^*$ with the denominator, the weights must alternate their sign for the rational function to have no poles in $[a, b]$. For this reason, the most simple weights, given in [2], are $v_j = (-1)^j$, i.e., the Lagrange basis functions are

$$\ell_j(x) = \frac{(-1)^j}{x - x_j} \bigg/ \sum_{k=0}^n \frac{(-1)^k}{x - x_k}. \quad (3.1)$$

This choice has several nice features:

- $r_n[f]$ does not have any real poles (for every distribution of the nodes);
- $r_n[f]$ is extremely well conditioned, as conjectured in [2]. For equispaced points, Bos, De Marchi and Hormann [17] proved that

$$\frac{2n}{4 + n\pi} \ln(n + 1) \leq A_n \leq 2 + \ln n.$$

This result has been improved in [18,19], but with a similar logarithmic pattern; it has also been extended to more general nodes in [20].

The only (but major) drawback of the weights in (3.1) is the slow convergence; it was conjectured in [2], and proved in [7], that it is $\mathcal{O}(h)$, where

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

A study of the rational trigonometric case in [2] led the author to the introduction of a second set of weights, which for a closed interval read

$$v_j = (-1)^j \delta_j, \quad \delta_j = \begin{cases} 1/2, & j = 0 \text{ or } j = n, \\ 1, & \text{otherwise.} \end{cases}$$

The corresponding $r_n[f]$ again shows certain remarkable features:

- it does not have any poles in $[a, b]$;
- numerical results in [2] led to the conjecture of an extremely good condition;
- the conjecture in [16] of an $\mathcal{O}(h^2)$ -convergence has been proved for equispaced nodes in [7];
- it converges exponentially when the x_j are the Chebyshev points of the second kind, as it then coincides with the polynomial interpolant; this property is conserved with any conformal map of such nodes [16].

First numerical examples with large n are given in Table 1 of [2].

4. The family of Floater and Hormann interpolants

For a set of $n + 1$ strictly ordered nodes and $d \in \mathbb{N}^0$, $d \leq n$, Floater and Hormann give a denominator such that, for the corresponding $r_n[f]$,

$$\|f - r_n[f]\| = \mathcal{O}(h^{d+1}).$$

They obtain this property by considering $n - d + 1$ polynomials p_j , each of which interpolates $d + 1$ consecutive values of f ; more precisely, p_j is the polynomial of degree at most d interpolating $f_j, f_{j+1}, \dots, f_{j+d}$. The original form of the rational interpolants (one for every d) then is

$$r_n[f](x) = \sum_{j=0}^{n-d} \lambda_j(x) p_j(x) \Big/ \sum_{j=0}^{n-d} \lambda_j(x), \quad \text{where } \lambda_j(x) = \frac{(-1)^j}{(x - x_j) \cdots (x - x_{j+d})}.$$

Theorem 4.1 ([7]). *For every admissible d , $r_n[f]$ interpolates f at the given nodes and has no poles in \mathbb{R} .*

The zeros and the poles of rational interpolants can be computed from their barycentric form through companion matrices, see, e.g., [21].

Following Lemma 2.1, Floater and Hormann give the barycentric weights of their interpolant for general nodes,

$$v_j = \sum_{i \in J_j} (-1)^i \prod_{k=i, k \neq j}^{i+d} \frac{1}{x_j - x_k}, \quad J_j := \{i \in \{0, \dots, n\} : j - d \leq i \leq j\}.$$

The v_j oscillate in sign; for *equispaced* nodes, their absolute values are

$$\begin{array}{ll} 1, & 1, & 1, & 1, & 1, \dots, 1, & 1, & 1, & 1, & 1 & d = 0 & [2] \\ \frac{1}{2}, & 1, & 1, & 1, & 1, \dots, 1, & 1, & 1, & 1, & \frac{1}{2} & d = 1 & [2] \\ \frac{1}{4}, & \frac{3}{4}, & 1, & 1, & 1, \dots, 1, & 1, & 1, & \frac{1}{4}, & \frac{3}{4} & d = 2 & [7] \\ \frac{1}{8}, & \frac{4}{8}, & \frac{7}{8}, & 1, & 1, \dots, 1, & 1, & \frac{7}{8}, & \frac{4}{8}, & \frac{1}{8} & d = 3 & [7]. \end{array}$$

Notice that the second interpolant coincides with the one given in [2] for equispaced points only: otherwise the weights differ.

The convergence is algebraic with power $d + 1$:

Theorem 4.2 ([7]). Let $1 \leq d \leq n$ and $f \in C^{d+2}[a, b]$. Then

– if $n - d$ is odd,

$$\|r_n[f] - f\| \leq (b - a) \frac{\|f^{(d+2)}\|}{d + 2} h^{d+1};$$

– if $n - d$ is even,

$$\|r_n[f] - f\| \leq \left((b - a) \frac{\|f^{(d+2)}\|}{d + 2} + \frac{\|f^{(d+1)}\|}{d + 1} \right) h^{d+1}.$$

Much is already known about the condition of this Floater–Hormann scheme: for equispaced points, Bos, De Marchi, Hormann, and the second author [22] have shown that

$$\frac{2^{d-2}}{d+1} \ln \left(\frac{n}{d} - 1 \right) \leq \Lambda_n \leq 2^{d-1} (2 + \ln n) : \quad (4.1)$$

the Lebesgue constant grows logarithmically with n , but *exponentially* with d .

In practice, one may choose an arbitrarily high order $d + 1$ of convergence only with n much larger than d . The choice of the optimal d for a given finite n is not a trivial task. Güttel and the second author [23] have cleared up the case when f is analytic in a domain containing the interval of interpolation.

Suppose that the parameter $d(n)$ is a *variable* nonnegative integer such that $d(n)/n \rightarrow C$ as $n \rightarrow \infty$, for $C \in (0, 1]$ fixed. In practice, e.g., $d(n) = \text{round}(Cn)$.

Theorem 4.3 ([23]). Let f be a function analytic in an open neighborhood of $[a, b]$ and $R > 0$ the smallest number such that f is analytic in the interior of a certain contour \mathcal{C}_R determined by C and the distribution of the nodes. Then

$$\limsup_{n \rightarrow \infty} \|f - r_n\|^{1/n} \leq R.$$

The authors have also suggested a procedure for the practical choice of C (which automatically leads to a choice of d) as a function of n in order to balance the growth of Λ_n . They notice that

$$\begin{aligned} \text{effective numerical error} &\approx \text{interpolation error in exact arithmetic} + \text{imprecision} \times \text{condition number} \\ &\lesssim DR^n + \varepsilon \|f\| \Lambda_n \\ &=: \text{predicted error,} \end{aligned}$$

where D is a constant depending on f and ε the unit roundoff. Then, given n and the singularity of f closest to $[a, b]$ with respect to \mathcal{C}_R , they determine $d(n) \in \{0, \dots, n\}$ such that the predicted error is minimal.

Fig. 2 displays the results in an example, the interpolation of the function $\Gamma(x + 2)$ on the interval $[-1, 1]$, with the closest singularity at $x = -2$. All curves are functions of n : the top right picture gives C , the bottom right $d(n)$ and the left displays the obtained errors. The latter also shows the predicted error curve as a dashed line, as well as ε times Λ_n (or, rather, its bound as a function of d and n given in (4.1)) as a dotted line. One notices the initial exponential convergence for small n (for which $d = n$, meaning that the interpolating polynomial is used) and the almost uniform decay of the error up to about n times machine precision.

5. An extended family of barycentric rational interpolants

Consider equispaced points again, and a fixed d . By looking at the plots of the Lebesgue functions for the first values of d , some of which are given in Fig. 3 for $n = 40$, the second author has observed an interesting feature: the maxima of the downward opening curves between two consecutive nodes are large in at most d subintervals near each extremity. The idea has then germinated to try to eliminate these unstable stretches by extending the interpolation interval by dh on each side of $[a, b]$, constructing an interpolant on $[a - dh, b + dh]$ while still using it on $[a, b]$ only.

More precisely, $2d$ extra nodes x_{-d}, \dots, x_{-1} and x_{n+1}, \dots, x_{n+d} are considered, d on each side of the interval, and approximate values \tilde{f}_j of f at these nodes are computed by a discrete Taylor polynomial with derivatives approximated by (linear rational) finite differences (see Section 8) *using only the given values of f in $[a, b]$* . These finite differences are the derivatives of a member of the Floater–Hormann family with parameter \tilde{d} in the nodes $x_0, \dots, x_{\tilde{n}}$, resp. $x_{n-\tilde{n}}, \dots, x_n$, for an \tilde{n} much smaller than n . At the original nodes x_j , $j = 0, \dots, n$, the given f_j are used.

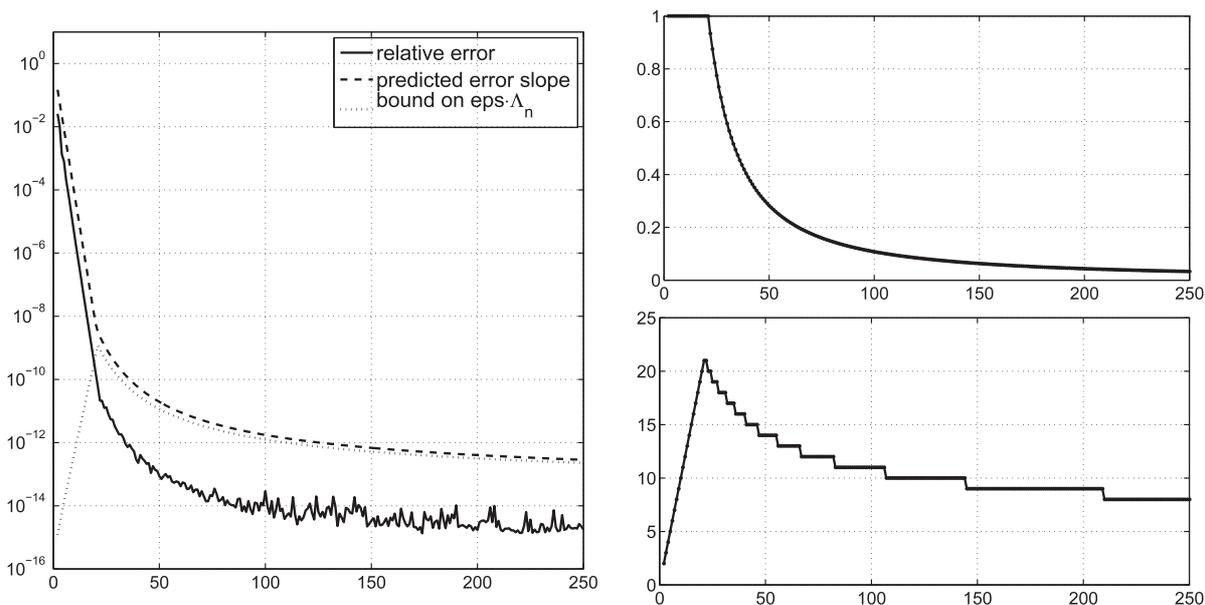


Fig. 2. Relative errors for the interpolation of $f(x) = \Gamma(x + 2)$ with $2 \leq n \leq 250$ equispaced nodes in $[-1, 1]$, $d(n) = \text{round}(Cn)$ and nearly optimal values of d .

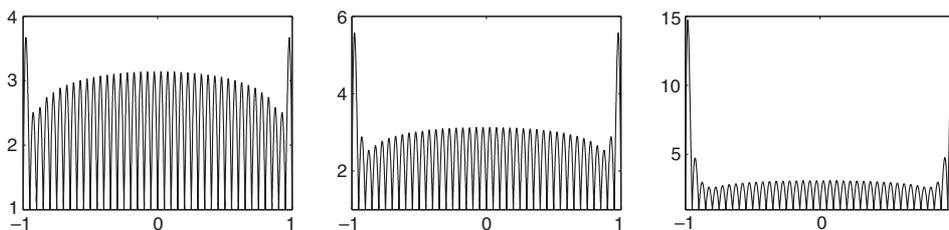


Fig. 3. Lebesgue functions for Floater–Hormann interpolation with equispaced nodes in $[-1, 1]$, $d = 2, 3, 5$ and $n = 40$.

The new interpolant is then computed from the global data with the Floater–Hormann weights for the extended set of nodes,

$$\tilde{r}_n[f](x) := \frac{\sum_{j=-d}^{n+d} \frac{\tilde{v}_j}{x - x_j} \tilde{f}_j}{\sum_{j=-d}^{n+d} \frac{\tilde{v}_j}{x - x_j}},$$

and evaluated only in $[a, b]$.

Theorem 5.1 ([24]). Suppose n, d, \tilde{n} and \tilde{d} are positive integers, $\tilde{d} \leq \tilde{n} < n$, and assume that $f \in C^{d+2}[a - dh, b + dh] \cap C^{2\tilde{d}+1}([a, a + \tilde{n}h] \cup [b - \tilde{n}h, b])$ is sampled at $n + 1$ equispaced nodes in $[a, b]$. Then

- (i) $\tilde{r}_n[f]$ has no real poles;
- (ii) for a constant K independent of n ,

$$\|\tilde{r}_n[f] - f\| \leq Kh^{\min(d, \tilde{d})+1},$$

- (iii) the associated Lebesgue constant $\tilde{\Lambda}_n$ grows logarithmically with n and d :

$$\tilde{\Lambda}_n \leq 2 + \ln(n + 2d).$$

The error with the extended family is often smaller than with the original one. Fig. 4 shows a comparison of the interpolation of Runge’s function $1/(1 + x^2)$ with the spline of order 5, the original Floater and Hormann interpolant with $d = 4$ and the member of the extended family with $d = 4, \tilde{n} = 11$ and $\tilde{d} = 7$, for $20 \leq n \leq 1000$.

At the extremities, the Lebesgue functions associated with the extended family are spectacularly better than those of the original family given in Fig. 3. As an example, the function $\tilde{\Lambda}$ with 51 nodes and $d = 3$ is given on the left of Fig. 5, where it is compared with the excellent ones of polynomial interpolation between Chebyshev nodes: $\tilde{\Lambda}_n$ is even smaller than the polynomial Λ_n of Chebyshev points! (The rightmost Λ is deceptive, as its extremal parts coincide with the verticals at ± 1 : in fact, Λ_n is larger for the points of the first kind than for those of the second, see [11, p. 8].)

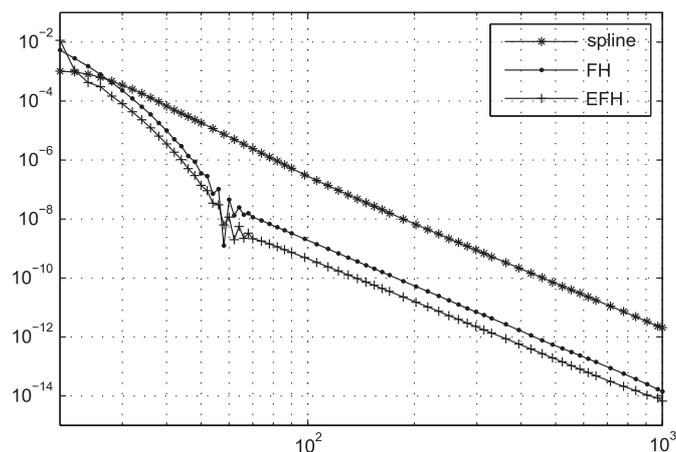


Fig. 4. Error comparison of spline, FH and EFH interpolation of $1/(1+x^2)$ with $d = 4$ and $20 \leq n \leq 1000$.

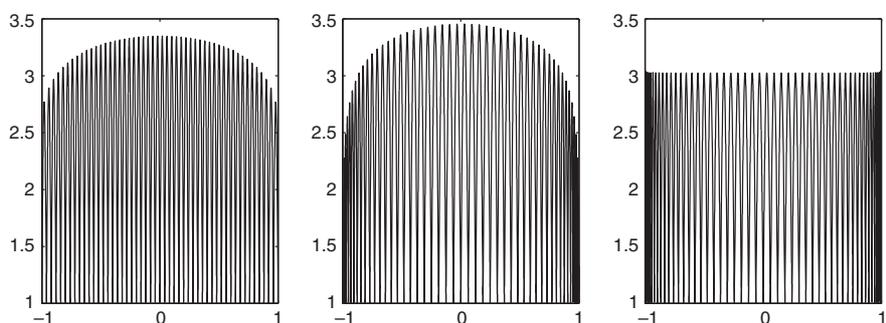


Fig. 5. Lebesgue functions with $n = 50$ associated with extended FH interpolation for equispaced nodes and $d = 3$ (left), polynomial interpolation with Chebyshev points of the second kind (center) and first kind (right).

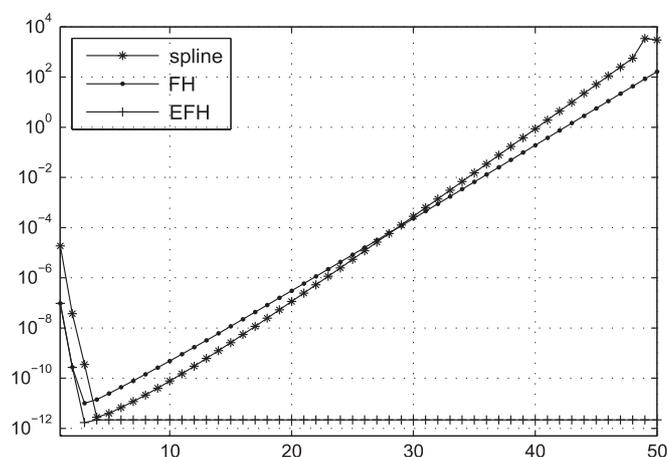


Fig. 6. Error comparison of spline, FH and EFH interpolation of $1/(1+x^2)$ with sign alternating 10^{-12} -perturbation, $n = 1000$ and $1 \leq d \leq 50$.

This nicer behavior of the Lebesgue constant has a decisive influence on the condition of the interpolation. In Fig. 6, the example of Fig. 4 is slightly modified by perturbing the f_j by a constant sequence of 10^{-12} with alternating signs; for a constant $n = 1000$, the figure displays the maximal error as a function of d , resp. of the order of the spline used as a comparison. In deep contrast with the two other tested interpolants, the perturbation has virtually no effect on $\tilde{r}_n[f]$!

As a conclusion to the description of these recent linear barycentric rational interpolants, we conjecture that they likely are very close to optimal for equispaced nodes. We have seen in Theorem 4.3 that for analytic functions the approximation error may decrease rapidly as a function of increasing, but still small, values of n . However, the schemes presented above

Table 1Error in the rational interpolation and the approximation of derivatives of $f(x) = 1/(1+x^2)$ in $[-5, 5]$ for $d = 3$ and equispaced nodes.

n	Interpolation		First derivative		Second derivative	
	Error	Order	Error	Order	Error	Order
10	6.9e-02		3.9e-01		1.5e+00	
20	2.8e-03	4.6	3.1e-02	3.7	2.6e-01	2.5
40	4.3e-06	9.4	7.8e-05	8.6	1.5e-03	7.4
80	5.1e-08	6.4	1.2e-06	6.0	6.1e-05	4.6
160	3.0e-09	4.1	1.0e-07	3.6	9.4e-06	2.7
320	1.8e-10	4.0	1.2e-08	3.1	1.2e-06	2.9
640	1.1e-11	4.0	1.5e-09	3.0	3.0e-07	2.0

all converge merely algebraically in the limit $n \rightarrow \infty$. One cannot expect much better approximations, at least for analytic functions. Indeed, Platte, Trefethen and Kuijlaars [25] have proved that an approximation of analytic functions from equispaced samples cannot be simultaneously exponentially convergent and well-conditioned.

6. Differentiation of barycentric rational interpolants

We now turn to some applications of the linear barycentric rational interpolants studied so far, starting with the approximation of derivatives. It has been known since the paper [26] by Schneider and Werner in 1986 that derivatives of rational interpolants written in barycentric form have very simple differentiation formulas. For the first derivative of $r_n[f]$, for instance, one has

$$r_n[f]'(x) = \sum_{j=0}^n \frac{v_j}{x-x_j} \frac{r_n[f](x) - f_j}{x-x_j} \bigg/ \sum_{j=0}^n \frac{v_j}{x-x_j}, \quad x \text{ not a node,}$$

$$r_n[f]'(x_i) = - \sum_{\substack{j=0 \\ j \neq i}}^n v_j f[x_i, x_j] / v_i, \quad i = 0, \dots, n.$$

For $x \in [a, b]$, we denote the error by

$$e(x) := f(x) - r_n[f](x).$$

Some results require the *mesh ratio*

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

Equipped with this, we are in the position of stating the following results.

Theorem 6.1 ([27]). *For the Floater–Hormann interpolants, $r_n[f]' \rightarrow f'$ as follows:*

- if $d \geq 1$ and if $f \in C^{d+3}[a, b]$, then

$$\|e'\| \leq Kh^d, \quad \text{if } d \geq 2,$$

$$\|e'\| \leq K(\beta + 1)h, \quad \text{if } d = 1;$$

- if $d \geq 2$ and if $f \in C^{d+4}[a, b]$, then

$$\|e''\| \leq K(\beta + 1)h^{d-1}, \quad \text{if } d \geq 3,$$

$$\|e''\| \leq K(\beta^2 + \beta + 1)h, \quad \text{if } d = 2.$$

In the above estimates, the constants K depend only on f , d and the interval length.

These theoretical orders are beautifully confirmed in practical computations. Table 1 displays errors obtained with Runge's function and $d = 3$ for various values of n , as well as the corresponding experimental convergence orders.

In [27], the derivatives obtained from these linear rational interpolants were also compared with those gathered from the cubic spline interpolant with not-a-knot end conditions. In Fig. 7, the errors delivered by the rational interpolant are given as solid lines, those corresponding to the spline as dashed lines. For each of the two, the error is smallest with the interpolant, and increases with the order of the derivatives (the lines corresponding to the latter are higher). The figure shows that the error with the spline is smaller up to about $n = 15$, which is not surprising in view of the damped oscillations of the spline, but for larger n the error becomes smaller with the rational interpolant.

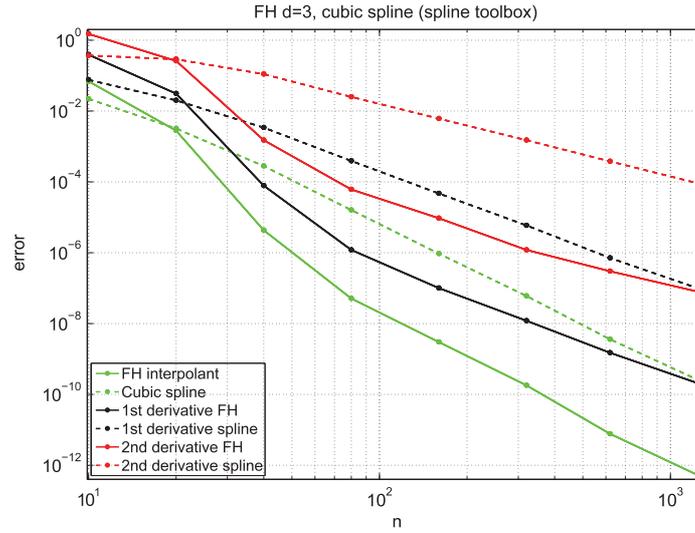


Fig. 7. Error comparison for f as in Table 1 and its first and second derivatives approximated by spline and linear rational interpolation.

7. Higher order derivatives at the nodes

Results have also been obtained for the convergence rate of higher order derivatives of $r_n[f]$ at equispaced and quasi-equispaced nodes. By *quasi-equispaced nodes* we mean points whose minimal spacing h_{\min} obeys

$$h_{\min} \geq ch,$$

where c is a constant.

Theorem 7.1 ([28]). *Suppose that $d \leq n, k \leq d$ and $f \in C^{d+1+k}[a, b]$. If the nodes are equispaced or quasi-equispaced and if f is approximated by the linear barycentric rational interpolation with Floater and Hormann weights, then*

$$|e^{(k)}(x_j)| \leq Kh^{d+1-k}, \quad 0 \leq j \leq n,$$

where K only depends on d, k and derivatives of f .

8. Differentiation matrices and rational finite differences

Differentiation matrices are important in several contexts, such as the solution of boundary value problems [1]. They may be obtained from the Lagrange representation

$$r_n[f] = \sum_{j=0}^n f_j \ell_j^{(v)}(x) \quad \text{with} \quad \ell_j^{(v)}(x) := \frac{v_j}{x - x_j} \bigg/ \sum_{k=0}^n \frac{v_k}{x - x_k} \quad (8.1)$$

of linear barycentric interpolants:

$$r_n[f]'(x) = \sum_{j=0}^n f_j \ell_j^{(v)'}(x), \quad r_n[f]''(x) = \sum_{j=0}^n f_j \ell_j^{(v)''}(x)$$

and

$$f'(x_i) \approx \sum_{j=0}^n D_{ij}^{(1)} f_j \quad \text{with} \quad D_{ij}^{(1)} := \ell_j^{(v)'}(x_i),$$

$$f''(x_i) \approx \sum_{j=0}^n D_{ij}^{(2)} f_j \quad \text{with} \quad D_{ij}^{(2)} := \ell_j^{(v)''}(x_i).$$

It turns out that the elements of the matrices $D^{(k)}$ satisfy a very simple recursion formula, starting with [16]

$$D_{ij}^{(1)} := \begin{cases} \frac{v_j}{v_i} \frac{1}{x_i - x_j}, & i \neq j, \\ -\sum_{\substack{\ell=0 \\ \ell \neq i}}^n D_{i\ell}^{(1)}, & i = j, \end{cases} \quad D_{ij}^{(2)} := \begin{cases} 2D_{ij}^{(1)} \left(D_{ii}^{(1)} - \frac{1}{x_i - x_j} \right), & i \neq j, \\ -\sum_{\substack{\ell=0 \\ \ell \neq i}}^n D_{i\ell}^{(2)}, & i = j, \end{cases} \quad (8.2)$$

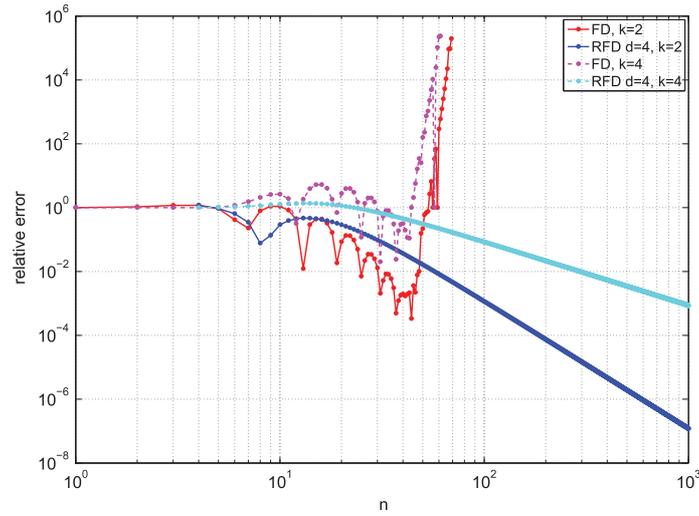


Fig. 8. Relative errors in the approximation at $x = 0$ of the second and fourth order derivatives of $1/(1 + x^2)$ sampled in $[0, 5]$.

and pursuing with [29,5]

$$D_{ij}^{(k)} := \begin{cases} \frac{k}{x_i - x_j} \left(\frac{v_j}{v_i} D_{ii}^{(k-1)} - D_{ij}^{(k-1)} \right), & i \neq j, \\ - \sum_{\substack{\ell=0 \\ \ell \neq i}}^n D_{i\ell}^{(k)}, & i = j. \end{cases}$$

With $\mathbf{f} := (f_0, \dots, f_n)^T$, the product $D^{(k)}\mathbf{f}$ returns the vector of the k th derivative of $r_n[f]$ at the nodes.

Derivatives of linear barycentric rational interpolants can also be used to construct *rational finite differences* for the approximation, at a node x_i , of the k th derivative of a function in C^{d+1+k} ,

$$f^{(k)}(x_i) \approx r_n^{(k)}[f](x_i) = \sum_{j=0}^n f_j \ell_j^{(v)(k)}(x_i),$$

where, again,

$$\ell_j^{(v)(k)}(x_i) = D_{ij}^{(k)}.$$

These differentiation weights, as well as the relation from the largest to the smallest of them, turn out to be much smaller than those of polynomial finite differences, in particular for one-sided derivatives; see [28]. The computation of derivatives by centered differences does not profit from this; but the approximation of one-sided derivatives by one-sided differences is more stable with rational ones than with their polynomial counterparts. Fig. 8 documents an example with Runge's function (FD designates polynomial finite differences, RFD rational ones).

9. Linear barycentric rational quadrature

When approximating the integral $I := \int_a^b f(x)dx$ of a real smooth function f sampled at $n + 1$ points by a linear quadrature rule $\sum_{k=0}^n w_k f_k$, one encounters two main situations:

- if the points may be chosen, Gauss or Clenshaw–Curtis quadrature can be used;
- if f is sampled at *equispaced* points, the Newton–Cotes rule is a viable solution for small n but, as it consists in the exact integration of the interpolating polynomial, becomes useless for n large: to stay with polynomial rules, one usually resorts to composite ones such as the trapezoidal rule, Simpson or Boole.

We now show how the replacement of polynomial by linear rational interpolation leads to quadrature formulas which allow arbitrarily large numbers of *equispaced* nodes. Clearly, every linear interpolation formula trivially yields a linear quadrature rule. For a barycentric rational interpolant, we have:

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

Table 2Error in the interpolation and the rational quadrature of $f(x) = \sin(100x) + 100$ for $d = 5$ with equispaced points in $[0, 1]$.

n	Interpolation		DRQ		IRQ	
	Error	Order	Error	Order	Error	Order
20	2.0e +00		6.8e -03		2.7e -03	
40	1.8e +00	0.2	1.4e -03	2.3	5.5e -02	-4.3
80	2.8e -02	6.0	9.0e -05	4.0	7.7e -04	6.2
160	6.6e -04	5.4	1.8e -07	9.0	5.7e -05	3.7
320	9.6e -06	6.1	5.7e -09	5.0	1.6e -06	5.2
640	1.3e -07	6.3	4.8e -11	6.9	3.4e -08	5.5
1280	1.1e -09	6.9	3.0e -13	7.3	7.3e -10	5.6

where

$$w_k := \int_a^b \frac{\frac{v_k}{x-x_k}}{\sum_{j=0}^n \frac{v_j}{x-x_j}} dx = \int_a^b \ell_k^{(v)}(x) dx.$$

For true rational interpolants whose denominator degree exceeds 4, there is no straightforward way of computing the integrals w_k . Two ideas for going around this difficulty are described in [30], a *direct* and an *indirect* one, which avoid expensive partial fraction decompositions and algebraic methods.

The *direct* rational quadrature rule (DRQ) is based on the stability of the rational interpolant and computes the w_k by well-behaved rules such as Gauss–Legendre or Clenshaw–Curtis. To fix the notation, let $w_k^{\mathcal{D}}$, $k = 0, \dots, n$, be so computed approximations of the w_k ; then the direct rational quadrature rule reads

$$I = \int_a^b f(x) dx \approx \sum_{k=0}^n w_k^{\mathcal{D}} f_k$$

instead of Q_n .

Theorem 9.1 ([30]). Suppose $d \in \mathbb{N}$, $d \leq n/2 - 1$, $f \in C^{d+3}[a, b]$ and $r_n[f]$ is the d th member of the Floater–Hormann family of linear rational interpolants with equispaced nodes. Assume further that the quadrature weights w_k in Q_n are approximated by a rule converging at least as $\mathcal{O}(h^{d+2})$. Then

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

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

Indirect quadrature approximates an antiderivative in the interval $[a, b]$ by a linear rational interpolant. For $x \in [a, b]$, one writes the problem

$$r_n[u](x) \approx \int_a^x f(y) dy$$

as an ordinary differential equation

$$r_n'[u](x) \approx f(x), \quad r_n[u](a) = 0$$

and collocate at the interpolation points.

As mentioned in Section 8, the first derivative of a rational interpolant at its nodes is

$$\mathbf{u}' = D\mathbf{u}, \quad u_j := r_n[u](x_j),$$

where $\mathbf{u} = (u_0, \dots, u_n)^T$ and $D_{ij} := D_{ij}^{(1)}$ is given in Eq. (8.2).

We then again set $\mathbf{f} = (f_0, \dots, f_n)^T$ and solve the system

$$D\mathbf{u} = \mathbf{f}, \quad \text{i.e., } \sum_{j=1}^n D_{ij} u_j = f_i, \quad i = 1, \dots, n.$$

The approximation u_n of the integral, which is called the indirect rational quadrature formula (IRQ), can be given by Cramer's rule; see [30].

Table 2 reports on computations with DRQ and IRQ for the function $f(x) = \sin(100x) + 100$ on the interval $[0, 1]$; it also includes the accuracy of $r_n[f]$ itself for the sake of comparison. The underlying linear rational interpolant uses $d = 5$, the weights in DRQ are computed by means of the Gauss–Legendre quadrature rule with 125 nodes. The experimental error of

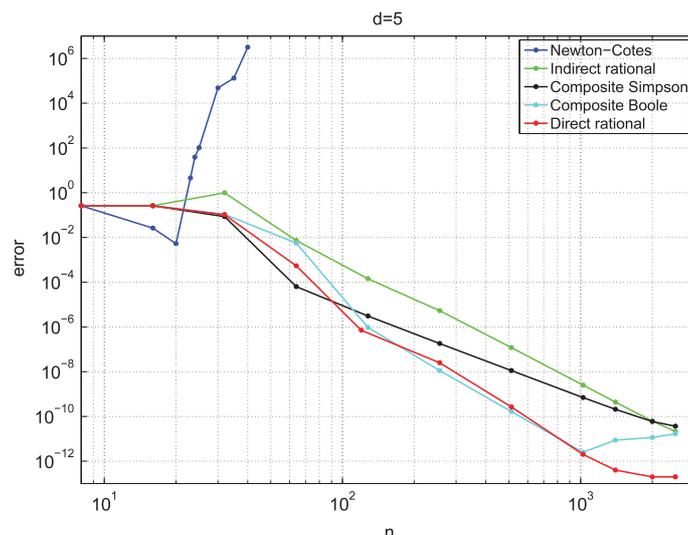


Fig. 9. Error comparison with five quadrature rules for f as in Table 2.

convergence of DRQ is about the $d + 2$ to be expected from the theorem, that of IRQ $d + 1/2$, half a unit less than that of the interpolant.

The same f is used for another comparison in Fig. 9, which gives the error as a function of n in a log–log representation. Besides the Newton–Cotes rules, which unsurprisingly yield disastrous results for n larger than about 20, DRQ and IRQ are compared with the two classical rules based on piecewise polynomial interpolation, composite Simpson and composite Boole. For small to moderate values of n , composite Simpson turns out to be the best rule. From about $n = 100$, it is surpassed by composite Boole and DRQ, which behave very similarly until $n = 1000$. However, DRQ eliminates the requirement inherent to composite Boole, that $n = 4k + 1$ for some $k \in \mathbb{N}$. This is an advantage, at least an aesthetic one, in some applications, so for instance the solution of Volterra integral equations by the quadrature method [31]. IRQ is the slowest converging rule, but one should remember that it is the only one giving not merely the value of I , but also the antiderivative of f at x_1, \dots, x_{n-1} , as u_1, \dots, u_{n-1} , and at all other $x \in [a, b]$, as the interpolant

$$r_n[u](x) = \sum_{j=0}^n \frac{v_j}{x - x_j} u_j / \sum_{j=0}^n \frac{v_j}{x - x_j} \approx \int_a^x f(y) dy, \quad x \in [a, b].$$

This approximate antiderivative is infinitely smooth.

We should point to another way of using linear rational interpolants in the approximation of antiderivatives and other calculations originating from an equispaced – or arbitrary – sample of a function [32]: one may approximate the rational interpolant $r_n[f]$ to those equispaced values by a chebfun and use the Chebfun system [33] to solve the problem at hand, e.g., find the antiderivative of $r_n[f]$. The solution is then given as a polynomial interpolant in Chebyshev points of the second kind, which can be easily evaluated in arbitrary points by the barycentric formula [34].

10. Conclusion

In this paper we have aimed at introducing the reader to linear barycentric rational interpolation and the various applications it has led to in recent years. We have pointed to its advantages over other infinitely smooth interpolants on a finite interval, mainly its simplicity, its proven good condition and its stability. The Ph.D. Thesis of the second author [32] provides further details. Our examples should also have made clear that there basically is no limit to the number of nodes that can be accommodated. As a final remark, we wish to emphasize the simple Lagrange representation $\sum_j f_j \ell_j^{(v)}(x)$ with the $\ell_j^{(v)}$ of (8.1): it allows for its straightforward use as an ansatz in the solution of functional equations and constitutes one further reason why we are confident that these interpolants will have a bright future in the solution of various problems in numerical analysis and scientific computing (see the very recent example in [35]).

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