Applications of linear barycentric rational interpolation at equispaced nodes

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Outline

Introduction and notation

Interpolation

One-dimensional interpolation problem

Given:

$$a \le x_0 < x_1 < \ldots < x_n \le b, \qquad n+1 \text{ distinct nodes and}$$
$$f(x_0), f(x_1), \ldots, f(x_n), \qquad \text{corresponding values.}$$

There exists a unique polynomial of degree $\le n$ that interpolates the f_i, i.e.

$$p_n[f](x_i) = f_i, \quad i = 0, 1, \ldots, n.$$

The Lagrange form of the polynomial interpolant is

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

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The first barycentric form

Denote the leading factors of the ℓ_j's by

$$\nu_j := \prod_{k \neq j} (x_j - x_k)^{-1}, \quad j = 0, 1, \ldots, n,$$

the so–called weights, which may be computed in advance.

Rewrite the polynomial in its first barycentric form

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

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- evaluation in $O(n)$ operations,
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The barycentric formula

The constant $f \equiv 1$ is represented exactly by its polynomial interpolant:

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

Dividing $p_n[f]$ by 1 and cancelling $L(x)$ gives

the barycentric form of the polynomial interpolant

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

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- **Interpolation is guaranteed**:

$$\lim_{x \to x_k} \frac{\displaystyle\sum_{j=0}^{n} \frac{\widehat{\nu}_j}{x - x_j} f_j}{\displaystyle\sum_{j=0}^{n} \frac{\widehat{\nu}_j}{x - x_j}} = f_k.$$

- Simplification of the weights:
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Form polynomial to rational interpolation

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Lemma

Let $\{x_j\}$, $j = 0, 1, \ldots, n$, *be* $n+1$ *distinct nodes,* $\{f_j\}$ *corresponding real numbers and let* $\{v_j\}$ *be any nonzero real numbers. Then*

(a) *the rational function*

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

interpolates f_k *at* x_k*:* $\lim_{x \to x_k} r_n[f](x) = f_k$*;*

(b) *conversely, every rational interpolant of the* f_j *may be written in barycentric form for some weights* v_j*.*

Floater and Hormann interpolants

Weights suggested in B.(1988):

- $(-1)^i$;
- $1/2, 1, 1, \ldots, 1, 1, 1/2$ with oscillating sign.

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Construction presented by Floater and Hormann

- Choose an integer $d \in \{0, 1, \ldots, n\}$,
- define $p_j(x)$, the polynomial of degree $\leq d$ interpolating $f_j, f_{j+1}, \ldots, f_{j+d}$ for $j = 0, \ldots, n-d$.

The d-th interpolant is given by

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

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Barycentric weights

Write $r_n[f]$ in barycentric form

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

with the weights

$$v_j = \sum_{i \in J_j} \prod_{\ell=i,\ \ell \neq j}^{i+d} \frac{1}{x_j - x_\ell}.$$

Barycentric weights

For equispaced nodes, the weights v_j oscillate in sign with absolute values

$$\begin{array}{rll}
1, 1, \ldots, 1, 1, & d = 0, & \text{(B.)} \\
\frac{1}{2}, 1, 1, \ldots, 1, 1, \frac{1}{2}, & d = 1, & \text{(B.)} \\
\frac{1}{4}, \frac{3}{4}, 1, 1, \ldots, 1, 1, \frac{3}{4}, \frac{1}{4}, & d = 2, & \text{(Floater-Hormann)} \\
\frac{1}{8}, \frac{4}{8}, \frac{7}{8}, 1, 1, \ldots, 1, 1, \frac{7}{8}, \frac{4}{8}, \frac{1}{8}, & d = 3. & \text{(Floater-Hormann)}
\end{array}$$

Theorem (Floater-Hormann (2007))

Let $0 \le d \le n$ *and* $f \in C^{d+2}[a,b]$, $h := \max_{0\le i\le n-1}(x_{i+1}-x_i)$, *then*

- *the rational function* $r_n[f]$ *has no poles in* $\mathbb{R}$,
- *if* $n-d$ *is odd, then*

$$\|r_n[f]-f\| \le h^{d+1}(b-a)\frac{\|f^{(d+2)}\|}{d+2} \qquad \text{if } d \ge 1,$$
$$\|r_n[f]-f\| \le h(1+\beta)(b-a)\frac{\|f''\|}{2} \qquad \text{if } d = 0;$$

- *if* $n-d$ *is even, then*

$$\|r_n[f]-f\| \le h^{d+1}\Big((b-a)\frac{\|f^{(d+2)}\|}{d+2}+\frac{\|f^{(d+1)}\|}{d+1}\Big) \qquad \text{if } d \ge 1,$$
$$\|r_n[f]-f\| \le h(1+\beta)\Big((b-a)\frac{\|f''\|}{2}+\|f'\|\Big) \qquad \text{if } d = 0.$$

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

Differentiation of barycentric rational interpolants

Proposition (Schneider-Werner (1986))

Let $r_n[f]$ be a rational function given in its barycentric form with non vanishing weights. Assume that x is not a pole of $r_n[f]$. Then for $k \geq 1$

$$
\begin{aligned}
\frac{1}{k!} r_n^{(k)}[f](x) &= \frac{\displaystyle\sum_{j=0}^{n} \frac{v_j}{x - x_j} r_n[f][(x)^k, x_j]}{\displaystyle\sum_{j=0}^{n} \frac{v_j}{x - x_j}}, \quad x \text{ not a node}, \\
\frac{1}{k!} r_n^{(k)}[f](x_i) &= -\left(\sum_{\substack{j=0 \\ j \neq i}}^{n} v_j r_n[f][(x_i)^k, x_j] \right) \Big/ v_i, \quad i = 0, \ldots, n.
\end{aligned}
$$

Differentiation matrices

Define the matrices $D^{(1)}$ and $D^{(2)}$ (Baltensperger-B.-Noël (1999)):

$$D_{ij}^{(1)} := \begin{cases} \dfrac{v_j}{v_i} \dfrac{1}{x_i - x_j}, \\ -\displaystyle\sum_{\substack{k=0 \\ k\neq i}}^{n} D_{ik}^{(1)}; \end{cases} \qquad D_{ij}^{(2)} := \begin{cases} 2D_{ij}^{(1)}\left(D_{ii}^{(1)} - \dfrac{1}{x_i - x_j}\right), & i \neq j, \\ -\displaystyle\sum_{\substack{k=0 \\ k\neq i}}^{n} D_{ik}^{(2)}, & i = j. \end{cases}$$

If $\mathbf{f} := (f_0, \ldots, f_n)^T$, then

$$D^{(1)} \cdot \mathbf{f}, \text{ respectively } D^{(2)} \cdot \mathbf{f},$$

returns the vector of the first, respectively second, derivative of $r_n[f]$ at the nodes.

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Convergence rates for the derivatives

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

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

Theorem (B.-Floater-Klein)

At the nodes, we have

- *if $d \geq 0$ and if $f \in C^{d+2}[a, b]$, then*

$$|e'(x_j)| \leq Ch^d, \quad j = 0, 1, \ldots, n;$$

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

$$|e''(x_j)| \leq Ch^{d-1}, \quad j = 0, 1, \ldots, n.$$

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Theorem (B.-Floater-Klein) (continued)

With the intermediate points, we have

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

$$\|e'\| \leq Ch^d \qquad \text{if } d \geq 2,$$
$$\|e'\| \leq C(\beta+1)h \qquad \text{if } d = 1;$$

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

$$\|e''\| \leq C(\beta+1)h^{d-1} \qquad \text{if } d \geq 3,$$
$$\|e''\| \leq C(\beta^2+\beta+1)h \qquad \text{if } d = 2.$$

Mesh ratio

$$\beta := \max\left\{\max_{1\leq i\leq n-1} \frac{|x_i - x_{i+1}|}{|x_i - x_{i-1}|}, \max_{0\leq i\leq n-2} \frac{|x_{i+1} - x_i|}{|x_{i+1} - x_{i+2}|}\right\}.$$

Remarks

- In the important cases $k = 1, 2$ the convergence rate of the k-th derivative is $O(h^{d+1-k})$ as $h \to 0$:
  In short:

  Loss of one order per differentiation.

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Runge's function

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

	Interpolation		First derivative		Second derivative	
n	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
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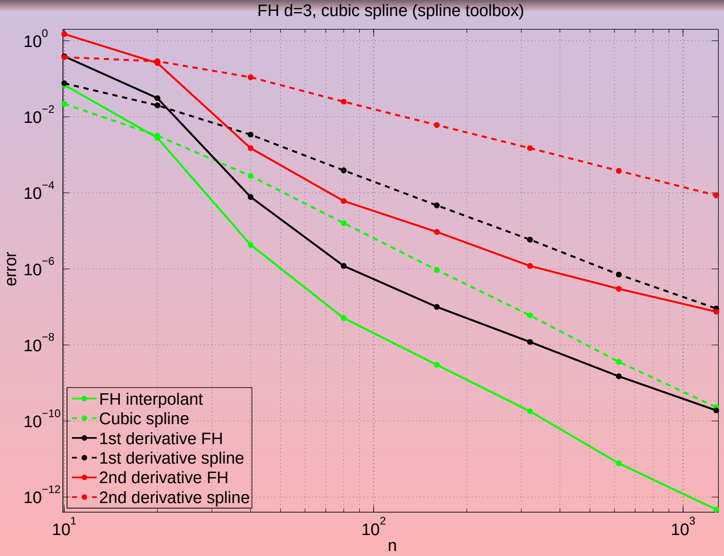
Comparison with cubic spline



Higher order derivatives and application to rational finite differences

Quasi-equispaced nodes

Let us now investigate the convergence rate of the k-th derivative, $k = 1, \ldots, d+1$, of $r_n[f]$ at equispaced or quasi-equispaced nodes. By quasi-equispaced nodes (Elling 2007) we shall mean here points whose minimal spacing $h_{\min}$ satisfies

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

where c is a constant.

Convergence rates for higher order derivatives

Theorem

Suppose n, d, $d \le n$, and k, $k \le d+1$, are positive integers and $f \in C^{d+1+k}[a,b]$. If the nodes x_j, $j = 0, \dots, n$, are equispaced or quasi-equispaced, then

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

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

Rational finite differences (RFD)

Let us introduce **rational finite difference** (RFD) formulas for the approximation, at a node x_i, of the k-th derivative of a C^{d+1+k} function,

$$\left.\frac{d^k f}{dx^k}\right|_{x=x_i} \approx \left.\frac{d^k}{dx^k} r_n[f]\right|_{x=x_i} = \sum_{j=0}^{n} D_{ij}^{(k)} f_j,$$

where $D_{ij}^{(k)}$ is the k-th derivative of the j-th Lagrange fundamental rational function at the node x_i.

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Rational finite differences (RFD)

In order to establish formulas for the RFD weights $D_{ij}^{(k)}$, we use the differentiation matrix $D^{(1)}$ defined earlier for the first order derivative and the "hybrid formula" (Tee 2006),

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

for higher order derivatives.

Weights for the first centered RFD formulas

Table: Weights for $\mathbf{d} = \mathbf{4}$ for the approximation of the 2-nd and 4-th order derivatives at $x = 0$ on an equispaced grid.

-4	-3	-2	-1	0	1	2	3	4
2nd derivative (order 3)								
		$-\frac{1}{12}$	$\frac{4}{3}$	$-\frac{5}{2}$	$\frac{4}{3}$	$-\frac{1}{12}$		
	$\frac{1}{63}$	$-\frac{5}{28}$	$\frac{11}{7}$	$-\frac{355}{126}$	$\frac{11}{7}$	$-\frac{5}{28}$	$\frac{1}{63}$	
$-\frac{1}{128}$	$\frac{5}{72}$	$-\frac{11}{32}$	$\frac{15}{8}$	$-\frac{1835}{576}$	$\frac{15}{8}$	$-\frac{11}{32}$	$\frac{5}{72}$	$-\frac{1}{128}$
4th derivative (order 1)								
		1	-4	6	-4	1		
	$-\frac{109}{441}$	$\frac{365}{147}$	$-\frac{1133}{147}$	$\frac{4826}{441}$	$-\frac{1133}{147}$	$\frac{365}{147}$	$-\frac{109}{441}$	
$\frac{1763}{12288}$	$-\frac{2845}{2304}$	$\frac{17017}{3072}$	$-\frac{3415}{256}$	$\frac{327787}{18432}$	$-\frac{3415}{256}$	$\frac{17017}{3072}$	$-\frac{2845}{2304}$	$\frac{1763}{12288}$

Weights for the first one-sided RFD formulas

Table: Weights for $\mathbf{d} = \mathbf{4}$ for the approximation of the 2-nd and 4-th order derivatives at $x = 0$ on an equispaced grid.

0	1	2	3	4	5	6	7	8
2nd derivative (order 3)								
$\frac{35}{12}$	$-\frac{26}{3}$	$\frac{19}{2}$	$-\frac{14}{3}$	$\frac{11}{12}$				
$\frac{15}{4}$	$-\frac{77}{6}$	$\frac{107}{6}$	-13	$\frac{61}{12}$	$-\frac{5}{6}$			
$\frac{319}{90}$	$-\frac{25}{2}$	$\frac{77}{4}$	$-\frac{161}{9}$	11	$-\frac{41}{10}$	$\frac{25}{36}$		
$\frac{379}{105}$	$-\frac{529}{42}$	$\frac{8129}{420}$	$-\frac{809}{42}$	$\frac{211}{14}$	$-\frac{1903}{210}$	$\frac{293}{84}$	$-\frac{127}{210}$	
$\frac{42143}{11760}$	$-\frac{1055}{84}$	$\frac{3245}{168}$	$-\frac{1615}{84}$	$\frac{337}{21}$	$-\frac{1727}{140}$	$\frac{429}{56}$	$-\frac{1775}{588}$	$\frac{179}{336}$
4th derivative (order 1)								
1	-4	6	-4	1				
3	-14	26	-24	11	-2			
$\frac{1774}{1125}$	$-\frac{83}{10}$	$\frac{2827}{150}$	$-\frac{5383}{225}$	$\frac{451}{25}$	$-\frac{5741}{750}$	$\frac{637}{450}$		
$\frac{9701}{4410}$	$-\frac{3127}{294}$	$\frac{33253}{1470}$	$-\frac{26069}{882}$	$\frac{2719}{98}$	$-\frac{27577}{1470}$	$\frac{6901}{882}$	$-\frac{2113}{1470}$	
$\frac{326620243}{172872000}$	$-\frac{785833}{82320}$	$\frac{17221193}{823200}$	$-\frac{6868019}{246960}$	$\frac{2892553}{102900}$	$-\frac{16757309}{686000}$	$\frac{40726213}{2469600}$	$-\frac{3976513}{576240}$	$\frac{2097749}{1646400}$

Weights for the first centered RFD formulas

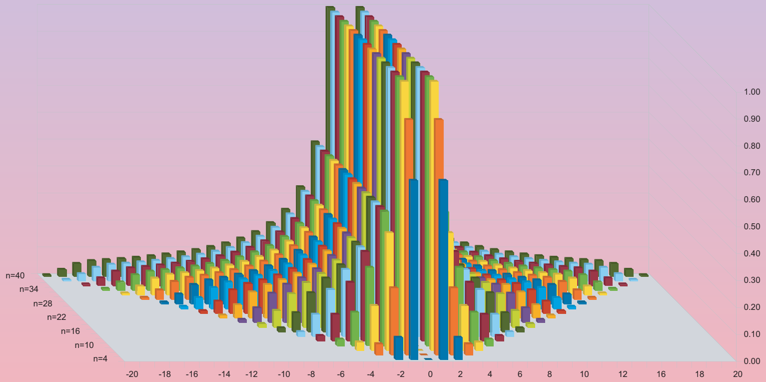

Figure: Absolute values of the weights for $\mathbf{d} = \mathbf{3}$ for the approximation of the first order derivative at $x = 0$ on an equispaced grid.

Weights for the first one-sided RFD formulas

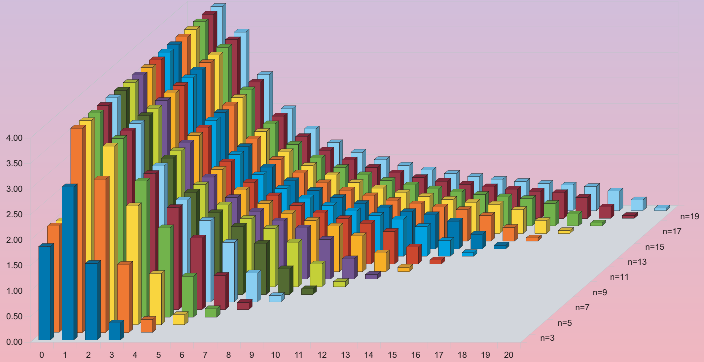

Figure: Absolute values of the weights for $\mathbf{d} = \mathbf{3}$ for the approximation of the first order derivative at $x = 0$ on an equispaced grid.

Relative errors in centered FD, resp. RFD for $d = 4$

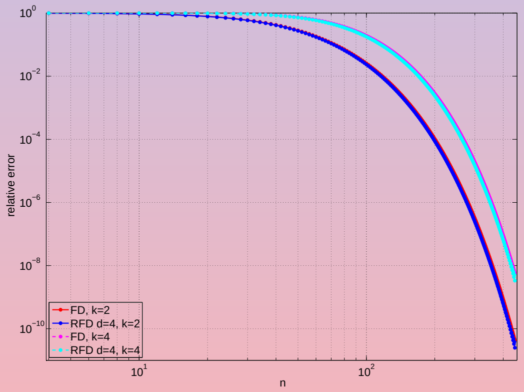

Figure: Relative errors in the approximation at $x = 0$ of the second and fourth order derivatives of $1/(1 + 25x^2)$ sampled in $[-5, 5]$.

Errors in one-sided FD, resp. RFD for $d = 4$

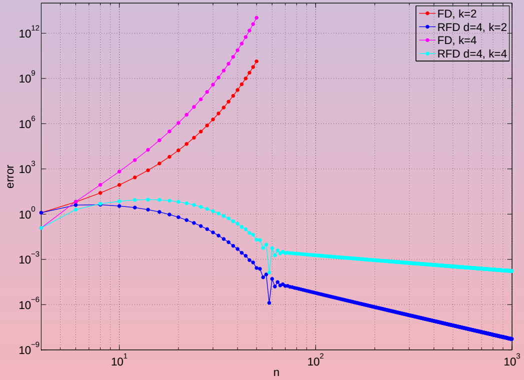

Figure: Errors in the approximation at $x = -5$ of the second and fourth order derivatives of $1/(1+x^2)$ sampled in $[-5, 5]$.

Integration of barycentric rational interpolants

Quadrature from equispaced samples

Problem: Given a real integrable function f sampled at $n+1$ points, approximate

$$I := \int_a^b f(x)dx$$

by a linear quadrature rule $\sum_{k=0}^{n} w_k f_k$, where $f_0, \ldots, f_n$ are the given data.

Two main situations:

- We can choose the points
  $\rightsquigarrow$ Gauss quadrature, Clenshaw-Curtis, ...
- f is sampled at $n+1$ equispaced points
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Integration of rational interpolants

Every linear interpolation formula trivially leads to a linear quadrature rule.

For a barycentric rational interpolant, we have:

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

$$= \sum_{k=0}^n w_k f_k =: Q_n,$$

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For true rational interpolants whose denominator degree exceeds 4, there is no straightforward way to establish a linear rational quadrature rule.

We are describing two ideas on how to do this, a direct and an indirect one, avoiding expensive partial fraction decompositions and algebraic methods.

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We are describing two ideas on how to do this, a **direct** and an **indirect** one, avoiding expensive partial fraction decompositions and algebraic methods.

Direct rational quadrature (DRQ)

Direct rational quadrature rules are based on the numerical stability of the rational interpolant and on well-behaved quadrature rules such as Gauss-Legendre or Clenshaw-Curtis.

Let $w_k^{\mathcal{D}}$, $k = 0, \ldots, n$, be some approximations of the weights w_k in Q_n; then the direct rational quadrature rule reads

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Convergence and degree of precision of DRQ in general

Error in interpolation: $O(h^p)$,
error in the quadrature approximating $\int_a^b r_n[f](x)dx$: $O(h^q)$.
If $q \geq p$, then

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

Similar arguments hold for the degree of precision.

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Convergence rates of DRQ in a particular case

Theorem

Suppose n and d, $d \le n/2-1$, are nonnegative integers, $f \in C^{d+3}[a,b]$ and $r_n[f]$ belongs to the family of interpolants presented by Floater and Hormann, interpolating f at equispaced nodes. Let the quadrature weights w_k in Q_n be approximated by a quadrature rule converging at least at the rate of $O(h^{d+2})$. Then

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

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

Indirect rational quadrature (IRQ)

Indirect quadrature means that we approximate a primitive in the interval $[a, b]$ by a linear rational interpolant. For $x \in [a, b]$, we write the problem

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

as an ODE

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

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To this end we make use of the formula for the first derivative of a rational interpolant explained earlier, giving the vector $\mathbf{u}'$ of the first derivative of $r_n[u]$ at the interpolation points

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

where

$$D_{ij} := D_{ij}^{(1)} = \begin{cases} \dfrac{v_j}{v_i}\dfrac{1}{x_i - x_j}, & i \neq j, \\ -\displaystyle\sum_{\substack{k=0\\k\neq i}}^{n} D_{ik}^{(1)}, & i = j. \end{cases}$$

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Set $\mathbf{u} = (u_0, \ldots, u_n)^T$, $\mathbf{f} = (f_0, \ldots, f_n)^T$ and solve the system

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

The approximation u_n of the integral and thus the indirect rational quadrature formula may be given by Cramer's rule

$$u_n = \frac{1}{\det\left(\left(D_{ij}\right)_{1 \le i,j \le n}\right)} \sum_{k=1}^{n} \det \begin{pmatrix} & & 0 \\ & & \vdots \\ & & 0 \\ \left(D_{ij}\right)_{\substack{1 \le i \le n \\ 1 \le j \le n-1}} & & 1 \\ & & 0 \\ & & \vdots \\ & & 0 \end{pmatrix} f_k$$

$$=: \sum_{k=1}^{n} w_k^{\mathcal{I}} f_k.$$

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Results for $f(x) = \sin(100x) + 100$

Table: Error in the interpolation and the rational quadrature of $f(x) = \sin(100x) + 100$ for $\mathbf{d} = \mathbf{5}$ at equispaced points in $[0, 1]$ (computing the $w_k^{\mathcal{D}}$ by a Gauss-Legendre quadrature with 125 points).

	Interpolation		DRQ		IRQ	
n	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
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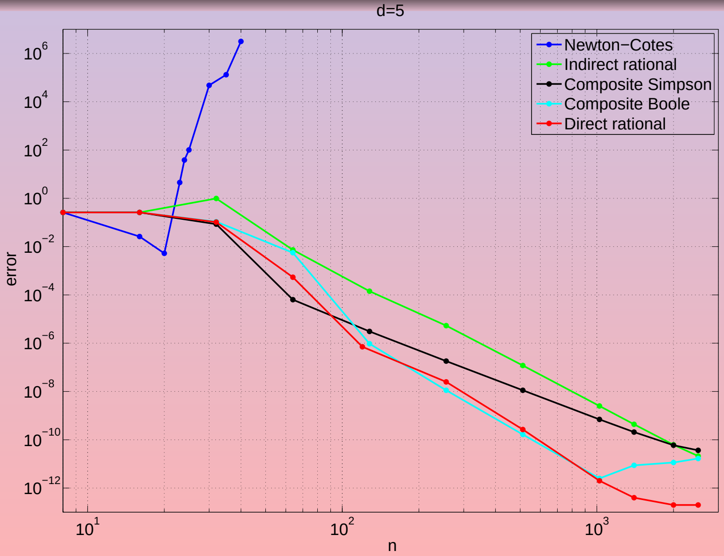
Comparison for $f(x) = \sin(100x) + 100$



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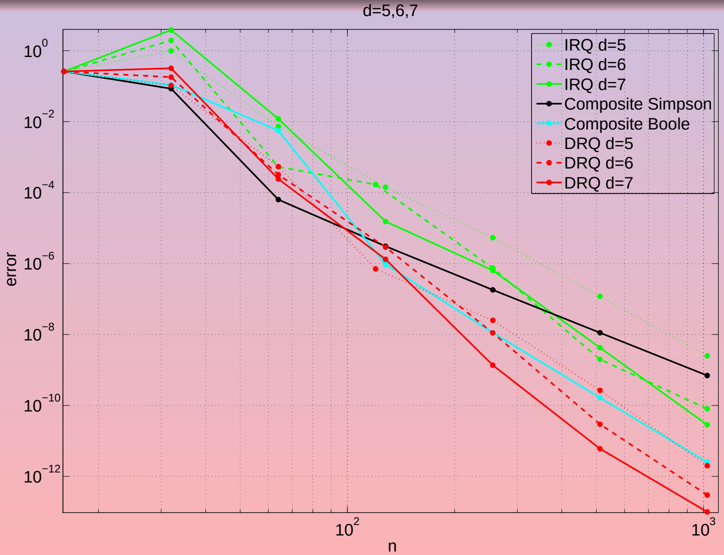

Note...

In contrast with DRQ, IRQ yields not only the value u_n approximating the integral, but also approximate values of the primitive $\int_a^x f(y)dy$ 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

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

This approximate primitive is infinitely smooth.

Thank you for your attention!