Applications of linear barycentric rational interpolation at equispaced nodes

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(with Georges Klein and Michael Floater)

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Outline

1. Interpolation
2. Differentiation of barycentric rational interpolants
3. Linear barycentric rational finite differences
4. Integration of barycentric rational interpolants
Introduction and notation

Interpolation

Berrut

Applications of LBR interpolation at equidistant nodes
One-dimensional interpolation problem

Given:

\[ a \leq x_0 < x_1 < \ldots < x_n \leq b, \quad n + 1 \text{ distinct nodes and corresponding values.} \]

There exists a unique polynomial of degree \( \leq n \) 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

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

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\[ f(x_0), f(x_1), \ldots, f(x_n), \quad \text{corresponding values}. \]

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The first barycentric form

Denote the leading factors of the $\ell_j$’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

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

where

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

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

- **Interpolation is guaranteed:**

  \[
  \lim_{x \to x_k} \frac{\sum_{j=0}^{n} \hat{\nu}_j (x - x_j)}{\sum_{j=0}^{n} \hat{\nu}_j} = f_k.
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- **Simplification of the weights:**
  Cancellation of common factor leads to simplified weights.
  For equispaced nodes,

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  \nu_j^* = (-1)^j \binom{n}{j}.
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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

\[
r_n[f](x) = \frac{\sum_{j=0}^{n} \frac{v_j}{x - x_j} f_j}{\sum_{j=0}^{n} v_j \frac{1}{x - x_j}},
\]

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.

Floater and Hormann in 2007: new choice for the weights
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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

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

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

\[
\begin{align*}
1, 1, \ldots, 1, 1, & \quad d = 0, \quad \text{(B.)} \\
\frac{1}{2}, 1, 1, \ldots, 1, 1, \frac{1}{2}, & \quad d = 1, \quad \text{(B.)} \\
\frac{1}{4}, \frac{3}{4}, 1, 1, \ldots, 1, 1, \frac{3}{4}, \frac{1}{4}, & \quad d = 2, \quad \text{(Floater-Hormann)} \\
\frac{1}{8}, \frac{4}{8}, \frac{7}{8}, 1, 1, \ldots, 1, 1, \frac{7}{8}, \frac{4}{8}, \frac{1}{8}, & \quad d = 3, \quad \text{(Floater-Hormann)}
\end{align*}
\]
Theorem (Floater-Hormann (2007))

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

- the rational function $r_n[f]$ has no poles in $\mathbb{R}$,
- if $n - d$ is odd, then
  $\|r_n[f] - f\| \leq h^{d+1}(b - a)\frac{\|f^{(d+2)}\|}{d+2}$ if $d \geq 1$,
  $\|r_n[f] - f\| \leq h(1 + \beta)(b - a)\frac{\|f''\|}{2}$ if $d = 0$;
- if $n - d$ is even, then
  $\|r_n[f] - f\| \leq h^{d+1}\left((b - a)\frac{\|f^{(d+2)}\|}{d+2} + \frac{\|f^{(d+1)}\|}{d+1}\right)$ if $d \geq 1$,
  $\|r_n[f] - f\| \leq h(1 + \beta)((b - a)\frac{\|f''\|}{2} + \|f'\|)$ if $d = 0$.

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

\[
\frac{1}{k!} r_n^{(k)}[f](x) = \frac{\sum_{j=0}^{n} v_j r_n[f][(x)^k, x_j]}{\sum_{j=0}^{n} v_j x - x_j}, \quad x \text{ not a node},
\]

\[
\frac{1}{k!} r_n^{(k)}[f](x_i) = -\left(\sum_{j=0}^{n} v_j r_n[f][(x_i)^k, x_j]\right)/v_i, \quad i = 0, \ldots, n.
\]
Define the matrices $D^{(1)}$ and $D^{(2)}$ (Baltensperger-B.-Noël (1999)):

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

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

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

returns the vector of the first, respectively second, derivative of $r_n[f]$ at the nodes.
Define the matrices $D^{(1)}$ and $D^{(2)}$ (Baltensperger-B.-Noël (1999)):

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

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

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  |e''(x_j)| \leq Ch^{d-1}, \quad j = 0, 1, \ldots, n.
  \]
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
  \[
  \| e' \| \leq Ch^d \quad \text{if } d \geq 2, \\
  \| e' \| \leq C(\beta + 1)h \quad \text{if } d = 1;
  \]

- if $d \geq 2$ and if $f \in C^{d+4}[a, b]$, then
  \[
  \| e'' \| \leq C(\beta + 1)h^{d-1} \quad \text{if } d \geq 3, \\
  \| e'' \| \leq C(\beta^2 + \beta + 1)h \quad \text{if } d = 2.
  \]

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\}.
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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.

Stricter conditions on the differentiability of $f$ compared to the interpolant.
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Remarks

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  In short:

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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 $d = 3$.

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Comparison with cubic spline

FH d=3, cubic spline (spline toolbox)

- FH interpolant
- 1st derivative FH
- 2nd derivative FH
- Cubic spline
- 1st derivative spline
- 2nd derivative spline

Error vs. n graph showing convergence rates for different methods.
Higher order derivatives and application to rational finite differences
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 \( n, d, d \leq n, \) and \( k, k \leq d + 1, \) are positive integers and \( f \in C^{d+1+k}[a, b]. \) If the nodes \( x_j, j = 0, \ldots, n, \) are equispaced or quasi-equispaced, then

\[
|e^{(k)}(x_j)| \leq C h^{d+1-k}, \quad 0 \leq j \leq n,
\]

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

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

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

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$$

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

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

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

for higher order derivatives.
Weights for the first centered RFD formulas

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

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<td>$\frac{1763}{12288}$</td>
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Weights for the first one-sided RFD formulas

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

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<td>4th derivative (order 1)</td>
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</table>
Figure: Absolute values of the weights for $d = 3$ 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 $d = 3$ 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
  \( \leadsto \) Gauss quadrature, Clenshaw-Curtis, ...

- \( f \) is sampled at \( n + 1 \) equispaced points
  \( \leadsto \) Newton-Cotes: unstable as \( n \to \infty \).
Quadrature from equispaced samples

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

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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:

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

where

\[
w_k := \int_a^b \frac{v_k}{x-x_k} \sum_{j=0}^n \frac{v_j}{x-x_j} \, dx.
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\[ = \sum_{k=0}^n w_k f_k =: Q_n, \]

where

\[ w_k := \int_a^b \frac{v_k}{\sum_{j=0}^n \frac{v_j}{x-x_j}} \, dx. \]
Our suggestions

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

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

instead of $Q_n$.
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\]

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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

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

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

Similar arguments hold for the degree of precision.
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Similar arguments hold for the degree of precision.
Convergence rates of DRQ in a particular case

**Theorem**

Suppose \( n \) and \( d, d \leq n/2 - 1 \), 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

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

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

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

and collocate at the interpolation points.
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Indirect rational quadrature (IRQ)

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

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

Remark: The matrix $D$ is centro-skew symmetric.
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\end{cases}
$$

Remark: The matrix $D$ is centro-skew symmetric.
Indirect rational quadrature (IRQ)

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

$$u_n = \frac{1}{\det \left( (D_{ij})_{1 \leq i, j \leq n} \right)} \sum_{k=1}^{n} \det \left( (D_{ij})_{1 \leq i \leq n}^{1 \leq j \leq n-1} \right) f_k$$

$$= \sum_{k=1}^{n} w_k^T f_k.$$
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The approximation \( u_n \) of the integral and thus the indirect rational quadrature formula may be given by Cramer's rule

\[
u_n = \frac{1}{\det \left( (D_{ij})_{1 \leq i, j \leq n} \right)} \sum_{k=1}^{n} \det \begin{pmatrix}
(D_{ij})_{1 \leq i \leq n, 1 \leq j \leq n-1} & 0 \\
0 & \ddots & 0 \\
0 & 0 & 1 \\
0 & \cdots & 0
\end{pmatrix} f_k
\]

\[
= \sum_{k=1}^{n} W_k \mathcal{I}_k f_k.
\]
Results for $f(x) = \sin(100x) + 100$

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

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

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<th>DRQ order</th>
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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 $d = 5$ at equispaced points in $[0, 1]$ (computing the $w_k^D$ by a Gauss-Legendre quadrature with 125 points).

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

- Newton–Cotes
- Indirect rational
- Composite Simpson
- Composite Boole
- Direct rational

Example:

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

d$=5,6,7$

![Graph showing comparison for $f(x) = \sin(100x) + 100$ for different values of $d$.](image)
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

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

This approximate primitive is infinitely smooth.
Thank you for your attention!