Efficient high-order rational integration and deferred correction with equispaced data

Georges Klein with Stefan Güttel

University of Oxford

Manchester, June 19, 2013

Outline

1. Introduction: linear barycentric rational interpolation
2. Integration
3. Rational deferred corrections (RDC)

Construction of **Floater–Hormann** interpolation for arbitrary nodes

- Given $n+1$ nodes, $a = x_0 < x_1 < \ldots < x_n = b$, and corresponding function values, $f_0, \ldots, f_n$, choose an integer $d \in \{0, 1, \ldots, n\}$, "**blending parameter**",
- for $i = 0, \ldots, n-d$, define $p_i(x)$, the polynomial of **low degree** $\leq d$ interpolating $f_i, f_{i+1}, \ldots, f_{i+d}$.

The d-th **interpolant** of the family is a "**blend**" of the $p_i(x)$,

$$r_n(x) = \frac{\displaystyle\sum_{i=0}^{n-d} \lambda_i(x) p_i(x)}{\displaystyle\sum_{i=0}^{n-d} \lambda_i(x)}, \quad \text{with} \quad \lambda_i(x) = \frac{(-1)^i}{(x-x_i)\ldots(x-x_{i+d})}.$$

Notice that for $d = n$, r_n simplifies to p_n.

Linear barycentric rational form

For its **evaluation**, we write r_n in *linear* **barycentric form**

$$r_n(x) = \frac{\displaystyle\sum_{i=0}^{n-d} \lambda_i(x) p_i(x)}{\displaystyle\sum_{i=0}^{n-d} \lambda_i(x)} = \frac{\displaystyle\sum_{i=0}^{n} \frac{w_i}{x - x_i} f_i}{\displaystyle\sum_{i=0}^{n} \frac{w_i}{x - x_i}}.$$

For **equispaced nodes**, the **weights** w_i do *not* depend on f, and oscillate in sign with absolute values

$$\begin{aligned}
&1, 1, \ldots, 1, 1, && d = 0,\\
&\tfrac{1}{2}, 1, 1, \ldots, 1, 1, \tfrac{1}{2}, && d = 1,\\
&\tfrac{1}{4}, \tfrac{3}{4}, 1, 1, \ldots, 1, 1, \tfrac{3}{4}, \tfrac{1}{4}, && d = 2,\\
&\tfrac{1}{8}, \tfrac{4}{8}, \tfrac{7}{8}, 1, 1, \ldots, 1, 1, \tfrac{7}{8}, \tfrac{4}{8}, \tfrac{1}{8}, && d = 3.
\end{aligned}$$

Lebesgue function and constant

The **Lebesgue constant** associated with linear barycentric interpolation,

$$\Lambda_{n,d} = \max_{a \le x \le b} \Lambda_{n,d}(x) = \max_{a \le x \le b} \sum_{i=0}^{n} \frac{|w_i|}{|x - x_i|} \Bigg/ \left| \sum_{i=0}^{n} \frac{w_i}{x - x_i} \right|,$$

is the **condition number** of the interpolation scheme.

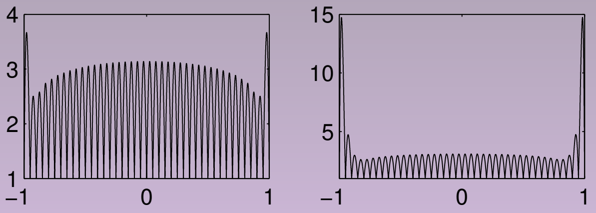


Figure: Lebesgue function for Floater–Hormann interpolation with equispaced nodes in $[-1, 1]$ with $d = 2$ and $d = 5$ and $n = 40$.

Lebesgue constant

Theorem (Bos–De Marchi–Hormann–K. '12)

Let $0 \leq d \leq n$ and the nodes x_i, $i = 0, \dots, n$, be equispaced. Then

$$\frac{2^{d-2}}{d+1} \log\left(\frac{n}{d} - 1\right) \leq \Lambda_{n,d} \leq 2^{d-1}(2 + \log n).$$

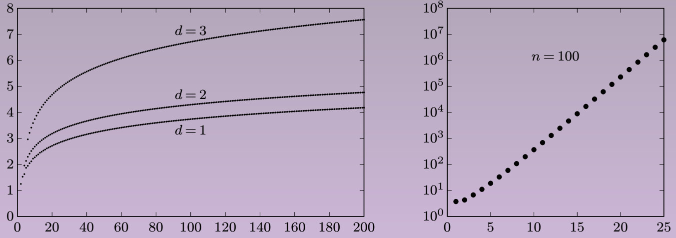


Figure: **Logarithmic growth** with n (left) and **exponential** with d (right).

Algebraic **convergence** and polynomial **reproduction**

Theorem (Floater–Hormann '07)

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

- $\|f - r_n\|_\infty \leq K h^{d+1}$,
  where K *depends only* d, $b - a$ *and derivatives of* f;
- *the analytic rational function* r_n *has no real poles;*
- r_n *reproduces polynomials of degree* $\leq d$ *if* $n - d$ *is even and of degree* $\leq d + 1$ *otherwise.*

Interpolation of **analytic** functions

If f is **analytic** inside a certain region of the complex plane, then the interpolation error may be written as

$$f(x) - r_n(x) = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{f(s)}{s - x} \cdot \frac{\sum_{i=0}^{n-d} \lambda_i(s)}{\sum_{i=0}^{n-d} \lambda_i(x)} \, \mathrm{d}s,$$

which is a **Hermite-type error formula**.

Analogy to polynomial interpolation:

$$f(x) - p_n(x) = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{f(s)}{s - x} \cdot \frac{\prod_{i=0}^{n} (x - x_i)}{\prod_{i=0}^{n} (s - x_i)} \, \mathrm{d}s.$$

Integration of rational interpolants

A linear interpolation formula leads to a **linear quadrature rule**. For a barycentric rational interpolant, we have:

$$I = \int_a^b f(x)\,\mathrm{d}x \approx \int_a^b r_n(x)\,\mathrm{d}x = \int_a^b \frac{\sum_{k=0}^n \frac{w_k}{x-x_k} f_k}{\sum_{j=0}^n \frac{w_j}{x-x_j}}\,\mathrm{d}x$$

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

where

$$\omega_k := \int_a^b \frac{\frac{w_k}{x-x_k}}{\sum_{j=0}^n \frac{w_j}{x-x_j}}\,\mathrm{d}x.$$

Direct rational integration (DRI)

Since the barycentric rational interpolant r_n is analytic, we may use any efficient scheme to approximate an **antiderivative** of r_n:

$$\int_a^x f(y)\,\mathrm{d}y \approx \int_a^x r_n(y)\,\mathrm{d}y.$$

Theorem (Güttel–K. '13)

Suppose n and d, $d \leq n/2-1$, are positive integers, $f \in C^{d+3}[a,b]$ and the nodes are equispaced. Then for any $x \in [a,b]$,

$$\left| \int_a^x f(y)\,\mathrm{d}y - \int_a^x r_n(y)\,\mathrm{d}y \right| \leq K h^{d+2}.$$

Error behavior with **fixed** d

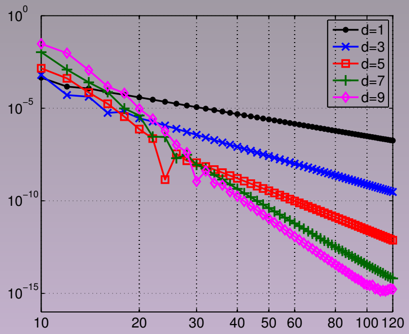


Figure: Errors in the approximation of antiderivatives of $1/(1+5x^2)$ from **equispaced** data on $[-1,1]$ with increasing n.

Iterated deferred correction

Rational deferred corrections (RDC)

Iterated deferred correction **principle**

We are interested in solving **initial-value problems** for a function $u : [0, T] \to \mathbb{C}^N$,

$$u'(t) = f(t, u(t)), \qquad u(0) = u_0 \in \mathbb{C}^N.$$

Picard reformulation to avoid numerical differentiation:

$$u(t) = u(0) + \int_0^t f(\tau, u(\tau))\, \mathrm{d}\tau.$$

Iterated deferred correction **principle**

Picard formulation:

$$u(t) = u(0) + \int_0^t f(\tau, u(\tau))\,\mathrm{d}\tau,$$

or equivalently, with $e = u - \widetilde{u}$ the approximation error,

$$\widetilde{u}(t) + e(t) = u(0) + \int_0^t f(\tau, \widetilde{u}(\tau) + e(\tau))\,\mathrm{d}\tau,$$

and the residual

$$r(t) = u(0) + \int_0^t f(\tau, \widetilde{u}(\tau))\,\mathrm{d}\tau - \widetilde{u}(t),$$

we obtain a **Picard-type formulation for the error**:

$$e(t) = r(t) + \int_0^t f(\tau, \widetilde{u}(\tau) + e(\tau)) - f(\tau, \widetilde{u}(\tau))\,\mathrm{d}\tau.$$

Rational deferred correction (RDC)

Method:

- solve $u(t) = u(0) + \int_0^t f(\tau, u(\tau))\,\mathrm{d}\tau$ with a **low order** method at **equally distributed** time steps $t_j \to \widetilde{u}$;
- compute the **residual** $r(t) = u(0) + \int_0^t f(\tau, \widetilde{u}(\tau))\,\mathrm{d}\tau - \widetilde{u}(t)$ with the **rational integration** scheme;
- use the same low order method for an **approximation of the error** $e(t) = r(t) + \int_0^t f(\tau, \widetilde{u}(\tau) + e(\tau)) - f(\tau, \widetilde{u}(\tau))\,\mathrm{d}\tau$;
- **correction**: $\widetilde{u}_{\mathrm{new}} = \widetilde{u} + e$;
- **iterate** $d + 1$ times or until desired accuracy is attained.

Possible extension: use Runge–Kutta instead of Euler.

Implicit-explicit combination

Semilinear initial value problem:

$$Mu'(t) = Ku(t) + g(t, u(t)), \quad u(0) = u_0,$$

where $M, K \in \mathbb{R}^{N \times N}$ are possibly large matrices, and g nonlinear.
Implicit-explicit Euler combination

$$Mu_{j+1} = Mu_j + h_j K u_{j+1} + h_j g(t_j, u_j), \quad h_j = t_{j+1} - t_j.$$

This recursion can be reformulated as

$$u_{j+1} = (M - h_j K)^{-1}(Mu_j + h_j g(t_j, u_j)),$$

which involves the solution of a linear system per time step.
Note: with **equally distributed** time steps $h_j = h$, only **one matrix inversion** is required.

Stability and accuracy regions

Dahlquist test equation on $[0, 1]$,

$$u'(t) = \lambda u(t), \qquad u(0) = 1.$$

Let $\widetilde{u}$ be the solution obtained with the method under consideration.

Stability region:

$$\{\lambda \in \mathbb{C} : |\widetilde{u}(1)| \leq 1\}.$$

Accuracy region:

$$\{\lambda \in \mathbb{C} : |u(1) - \widetilde{u}(1)| < \varepsilon\}.$$

Explicit time stepping with $n = 21$

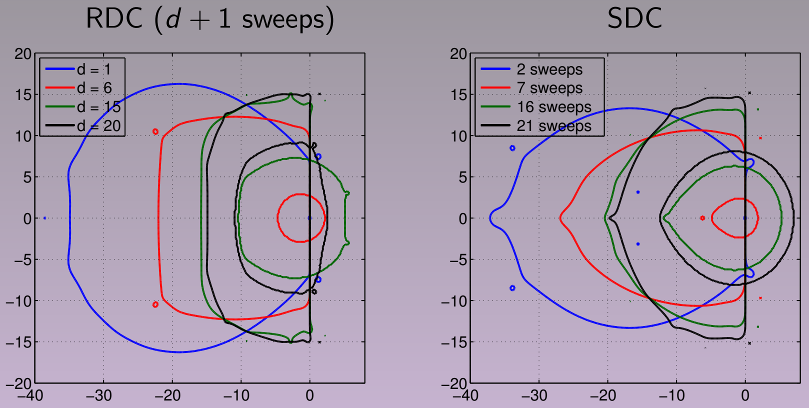


Figure: **Stability regions** (outer) and **accuracy regions** (inner) with target accuracy $\varepsilon = 10^{-8}$ with explicit Euler.

Implicit time stepping with $n = 20$

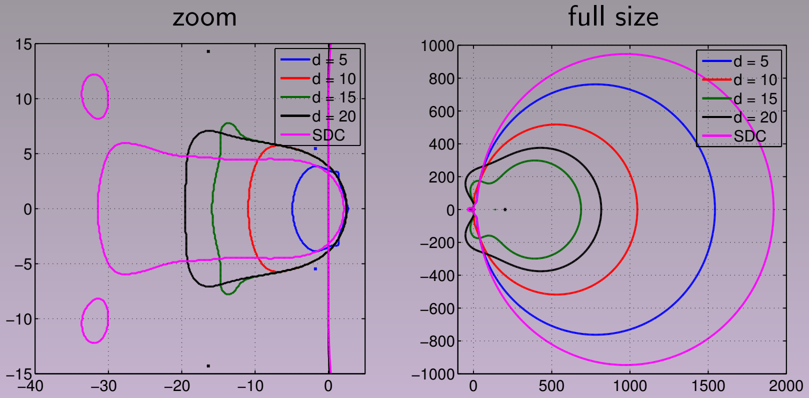
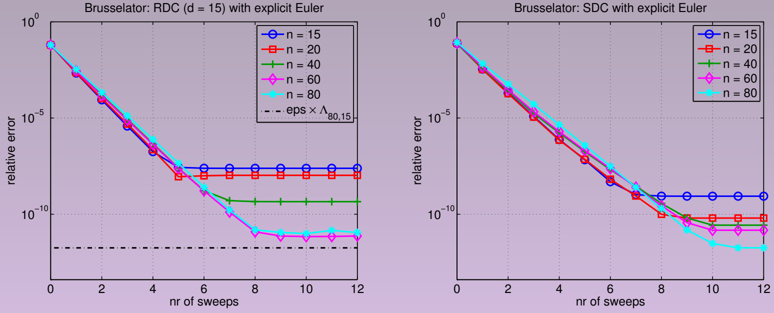


Figure: **Stability and accuracy regions** for RDC and SDC with implicit Euler, 8 sweeps, and target accuracy $\varepsilon = 10^{-7}$.

Brusselator

Brusselator problem for $t \in [0, 12]$,

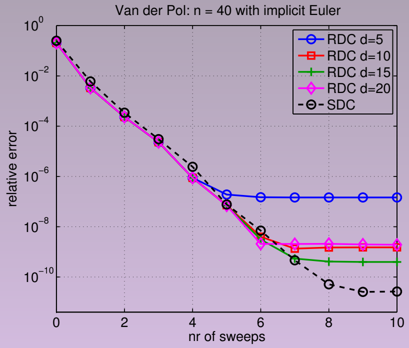
$$\begin{aligned} u_1'(t) &= 1 + u_1(t)^2 u_2(t) - 4u_1(t), \qquad & u_1(0) = 0, \\ u_2'(t) &= 3u_1(t) - u_1(t)^2 u_2(t), \qquad & u_2(0) = 1. \end{aligned}$$



Van der Pol equation

Van der Pol equation for $t \in [0, 10]$,

$$\begin{aligned} u_1'(t) &= u_2(t), & u_1(0) &= 2, \\ u_2'(t) &= 10(1 - u_1(t)^2)u_2(t) - u_1(t), & u_2(0) &= 0. \end{aligned}$$



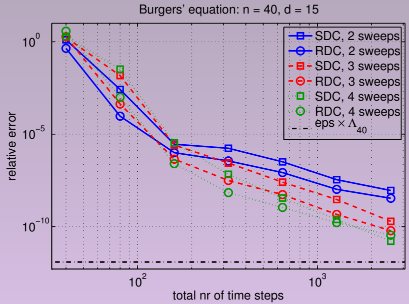
Burgers' equation

Burgers' equation for $u(t,x)$ defined on $[0,0.5]\times[-1,1]$

$$\partial_t u = 1/(100\pi)\,\partial_{xx}u - u\,\partial_x u,$$
$$u(t,-1)=u(t,1)=0,\quad u(0,x)=-\sin(\pi x).$$

Implicit-explicit reformulation wrt t_j

$$u_{j+1} = (I - h_j D_2)^{-1}(u_j + \frac{h_j}{2} D_1 u_j^2).$$



Summary

We have seen:

- linear barycentric rational interpolation;
- integration schemes based on rational interpolation;
- RDC.

Future work:

- combination with higher order integrators such as Runge–Kutta;
- parallelization, e.g., as in revisionist integral deferred correction; alternative: parareal.

Thank you for your attention!