Integrals via rational approximation

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Overview

A common task in science and engineering is to find the area under a curve. A *quadrature rule* is a method for estimating this area based on a small number of measurements of the curve's height. There is a wonderful connection between quadrature and rational functions (ratios of polynomials). With complex analysis, one can show that the difference between an exact integral $I = \int_{-1}^{1} f(x)\,dx$ and a numerical approximation $I_n = \sum_{j=1}^{n} f(x_j) w_j$ is given by

$$I - I_n = \frac{1}{2\pi i} \int_\Gamma f(z)(\phi(z) - r_n(z))dz, \tag{1}$$

where $\phi(z) = \log\frac{z+1}{z-1}$, r_n is the rational function $r_n(z) = \sum_j \frac{w_j}{z-x_j}$, and Γ is a path wrapping around $[-1,1]$ in the complex plane [3]. If we can approximate ϕ well by a rational function r, then the poles and residues of r will give an accurate quadrature rule. In fact, Gauss originally derived Gauss-Legendre quadrature, a state-of-the-art method, in this way. We present two new strategies for rationally approximating $\phi(z)$: Chebyshev-AAA and Multi-Point Padé approximation.

Chebyshev-AAA

https://www.overleaf.com/project/64bff116462d550ccff6b436 Inspired by the recent AAA algorithm [2], we propose a variant which we call Chebyshev-AAA. We look for a rational function in barycentric form:

$$r(z) = \left(\sum_j \frac{a_j w_j}{z - x_j}\right) \Big/ \left(\sum_j \frac{b_j w_j}{z - x_j}\right). \tag{2}$$

Here the x_j are points on a Chebyshev grid, and the w_j are the weights for polynomial interpolation. To find the unknowns a_j and b_j, we input a discrete set of sample points $Z \subset \mathbb{C}$, and minimize $\|d\phi - n\|_Z$ using linear algebra. Then, we find the poles and residues of $r(z)$, which are the nodes and weights of a new quadrature rule. The sample points z can be customized based on available information about $f(z)$, such as its singularities.

Multi-Point Padé

Suppose that $h(z)$ has known series expansions at 0 and ∞:

$$h(z) = c_0 + c_1 z + \ldots + c_n z^n + \cdots \tag{3}$$

$$h\left(\frac{1}{z}\right) = -\frac{c_{-1}}{z} - \frac{c_{-2}}{z^2} - \ldots - \frac{c_{-n}}{z^n} - \cdots \tag{4}$$

Then we can get a rational function approximating h by writing

$$r(z) = \frac{a_0 + a_1 z + \ldots + a_n z^n}{b_0 + b_1 z + \ldots + b_n z^n} \tag{5}$$

We cross-multiply (5) with (3) and (4) to get a matrix equation $Cb = 0$, where C is a Hankel matrix whose nullspace gives the unknowns b_i. We then use the b_i to find the a_i [1]. We cannot use $h = \phi$ directly because $\phi(z)$ is not analytic at 0, so we instead take $h = \phi \circ g$ where g is a M obius transform carrying 0 and ∞ to ω and $\overline{\omega}$, where $\omega \in \mathbb{C}$ is chosen near a singularity of the integrand f. This method works for values of n up to about 14 before numerical conditioning becomes an issue.

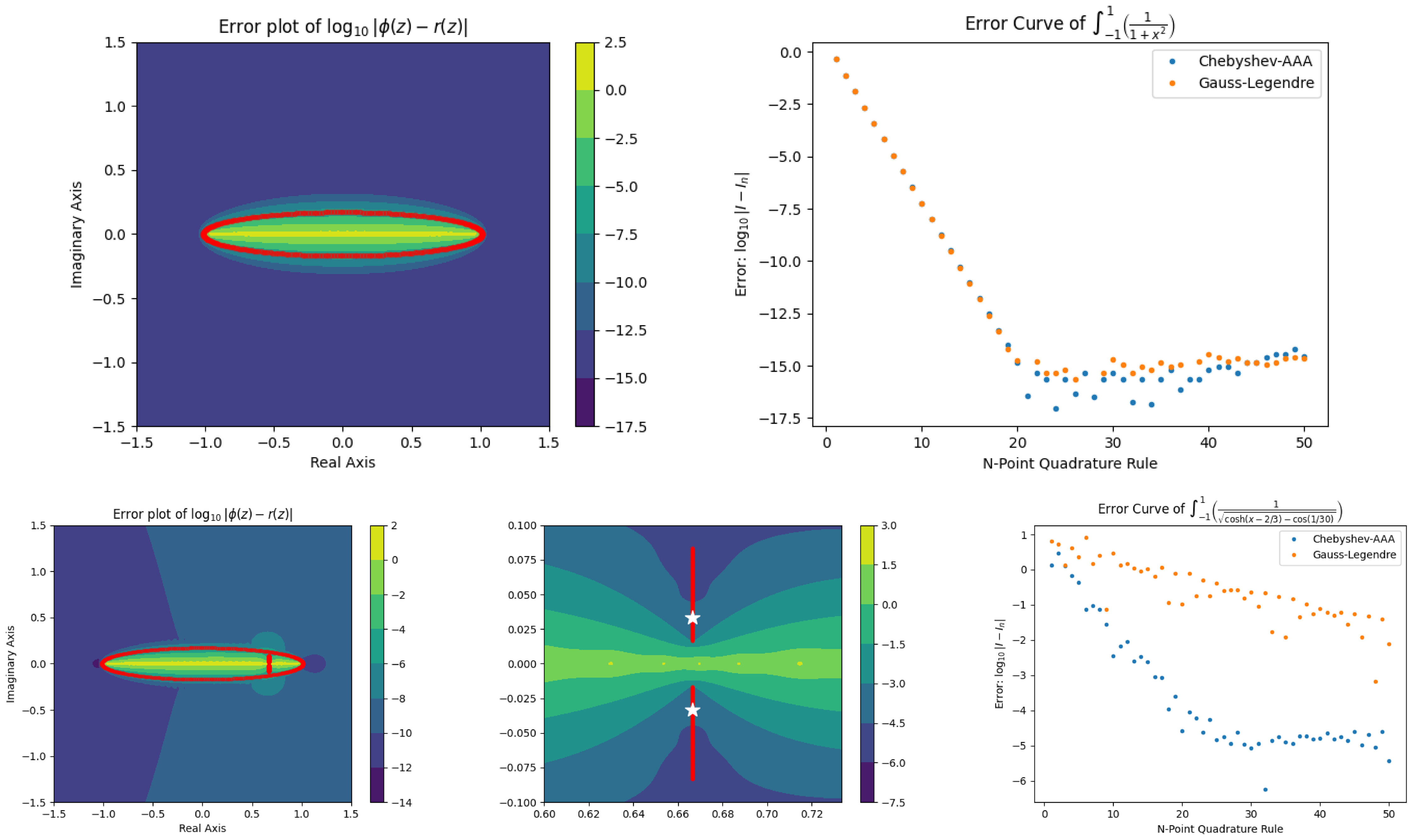

Figure 1:The performance of our Chebyshev-AAA method is similar to Gauss-Legendre quadrature for smooth functions (top row); we choose the sample points on an ellipse whose size shrinks as the quadrature order increases. For functions with a nearby singularity, we add additional sample points on a pair of segments, yielding a method that outperforms Gauss-Legendre quadrature (bottom row).

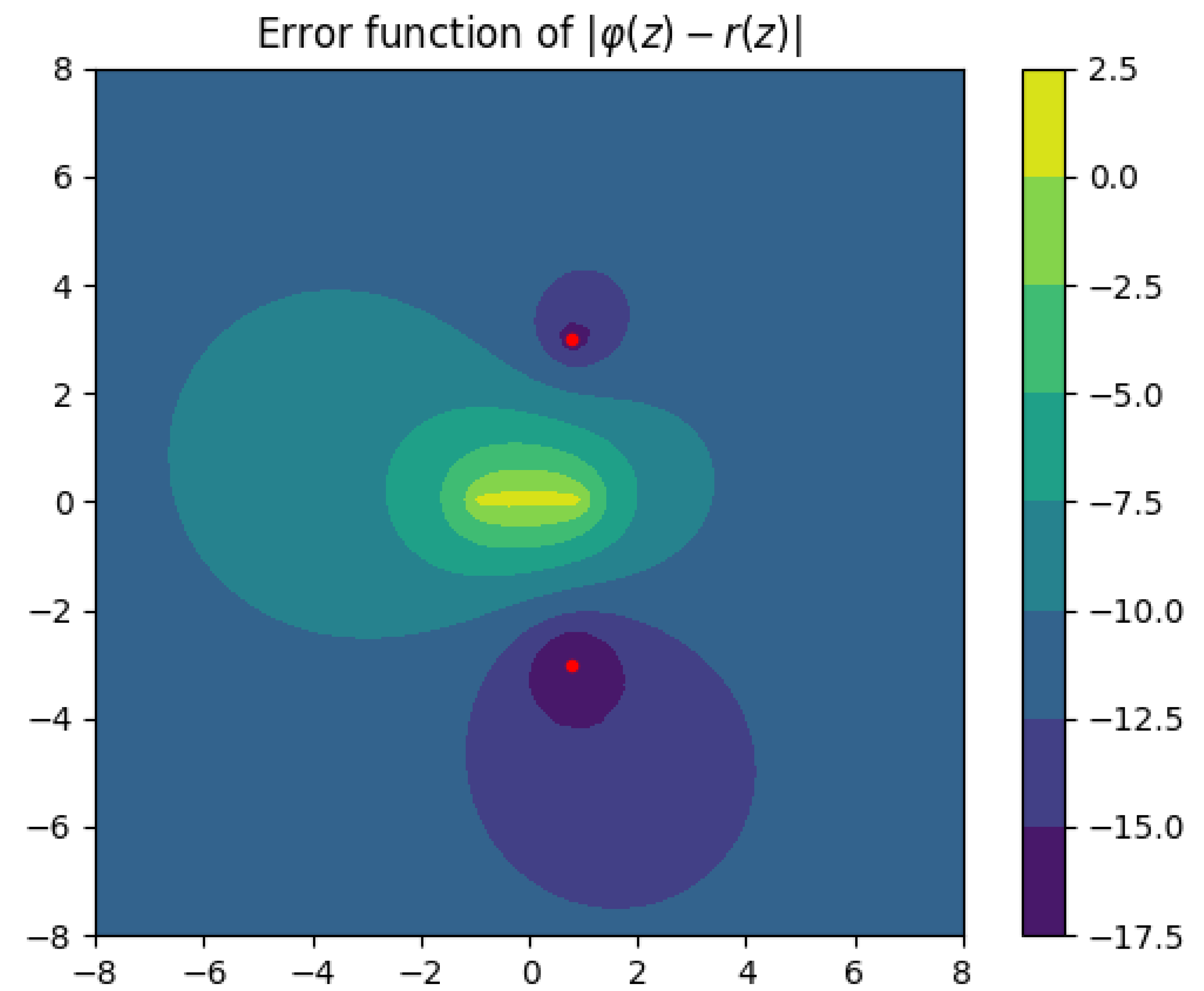

Figure 2:This figure shows the contour plot of $|\phi(z) - r(z)|$ where $r(z)$ comes from multi-point Padé approximation. The red dots $\omega = 0.8 + 3j$ and $\overline{\omega} = 0.8 - 3j$ are carried to 0 and ∞ by an initial Mobius transformation, so the approximation is best at these points. The zeros and poles of r cluster on $[-1,1]$ since ϕ has a branch cut discontinuity there.

References

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Acknowledgements

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