

QUADRATURE FORMULAS FROM RATIONAL APPROXIMATIONS*

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Abstract. It is shown that quadrature formulas in many different applications can be derived from rational approximation of the Cauchy transform of a weight function. Since rational approximation is now a routine technology, this provides an easy new method to derive all kinds of quadrature formulas as well as fundamental insight into the mathematics of quadrature. Intervals or curves of quadrature nodes correspond to near-optimal branch cuts of the Cauchy transform.

Key words. rational approximation, quadrature, AAA algorithm, Cauchy transform

MSC codes. 41A20, 65D32

1. Introduction. Quadrature formulas are used across scientific computing, and in numerical linear algebra, they have become an important tool for reducing large-scale eigenvalue and matrix function problems to small sets of matrix solves [3, 5, 7, 8, 9, 15, 21, 24, 25, 26, 30, 46, 48]. Traditionally they are derived and analyzed on a case-by-case basis. For one example, Gauss quadrature is connected with the theory of orthogonal polynomials [20]. For another, the exponentially convergent periodic trapezoidal rule is analyzed by discrete Fourier analysis or estimation of contour integrals [57]. More complicated quadrature problems are reduced to known ones such as these with the aid of conformal maps [25, 27, 28, 61], as in the “three Nicks” paper by Nick Higham, Nick Hale, and the second author [26] (see Figure 15).

In this article we show how quadrature formulas can be generated with very little effort by rational approximation, often approximation of functions with a “sign(z)” or “Zolotarev” flavor [33, 59]. The quadrature nodes are the poles of the rational function, delineating an approximate branch cut on a real interval or a complex contour, and the quadrature weights are the residues. This gives new insight into the mathematics of quadrature formulas. Until recently, there would have been few computational implications, because computation of rational approximations was a difficult problem, but with the appearance of the AAA (adaptive Antoulas–Anderson) algorithm in 2018 [42, 44], together with the AAA-Lawson enhancement to upgrade near-best to best [43], it has become routine. The Chebfun code `aaa.m`, which runs in MATLAB or Octave [13], is used for the examples of this paper, and AAA implementations are also available in Julia [12] and SciPy [60]. More recently another approximation algorithm due to Salazar Celis, based on Thiele continued fractions rather than barycentric representations, has also shown great promise [12, 49].

Section 2 lays out the mathematics of the connection between rational approximation and quadrature, and sections 3–7 and 9–10 apply these ideas to seven established quadrature problems, with section 8 summarizing certain necessary approximation matters related to Zolotarev. In each case, we first apply the rational approximation idea to a standard configuration and then we show how it can be modified to derive a quadrature formula for a variant problem. Section 11 closes the paper with a discussion.

We must say a word about our personal “journey.” Once the schema of section 2

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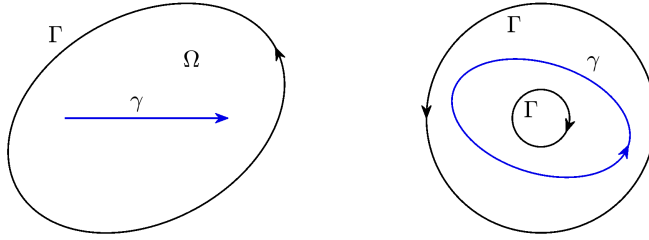


FIG. 1. On the left, sketch of an integration arc γ and a surrounding contour Γ in the complex plane. On the right, the analogous configuration for a closed integration contour γ .

became clear, it simply amazed us how, for one problem after another, we were able to use it to reproduce, with a fraction of a second of computing time, results won previously by careful analysis:

Figure 3: see Fig. 4.1 of [28],

Figure 4: see Fig. 1 of [52],

Figure 5: see Fig. 2.3 of [27],

Figure 9: see Fig. 3 of [10],

Figure 10: see Fig. 4.3 of [58],

Figure 11: see Fig. 1 of [61],

Figure 13: see Fig. 2 of [1],

Figure 16: see Fig. 2 of [26].

2. Mathematics of the approximation-quadrature connection. As on the left in Figure 1, let γ be a Jordan arc in the complex plane \mathbb{C} , that is, the image of $[-1, 1]$ under a real or complex homeomorphism. The simplest example is $[-1, 1]$ itself. Let $w(z)$ be an integrable weight function defined on γ , and suppose we are interested in approximating the integral

$$(2.1) \quad I = \int_{\gamma} f(z)w(z)dz.$$

Assume f is analytic in the closure of a Jordan region Ω containing γ , bounded by a Jordan curve Γ . By the Cauchy integral formula, we have

$$(2.2) \quad I = \int_{\gamma} \frac{1}{2\pi i} \left[\int_{\Gamma} \frac{f(s)ds}{s-z} \right] w(z)dz,$$

hence by exchanging orders of integration,

$$(2.3) \quad I = \frac{1}{2\pi i} \int_{\Gamma} f(s) \left[\int_{\gamma} \frac{w(z)dz}{s-z} \right] ds.$$

Let $\mathcal{C}(s)$ denote the function in square brackets, the *Cauchy transform* of w ,

$$(2.4) \quad \mathcal{C}(s) = \int_{\gamma} \frac{w(z)dz}{s-z},$$

which is analytic throughout $\mathbb{C} \cup \{\infty\} \setminus \gamma$. (This is also called the *Stieltjes transform*, and often there is a factor $1/(2\pi i)$ in front.) Then (2.3) becomes

$$(2.5) \quad I = \frac{1}{2\pi i} \int_{\Gamma} f(s) \mathcal{C}(s) ds,$$

and thus we have converted a real or complex integral over the arc γ to a complex contour integral over the enclosing contour Γ . Now suppose that r_n is a rational function of degree n that approximates \mathcal{C} on Γ . (A rational function of degree n is one that can be written as the ratio of two polynomials of degree at most n .) Then (2.5) suggests approximating I by

$$(2.6) \quad I_n = \frac{1}{2\pi i} \int_{\Gamma} f(s)r_n(s) ds.$$

Assume the poles of r_n are n distinct finite numbers z_1, \dots, z_n , so r_n can be written

$$(2.7) \quad r_n(s) = C + \sum_{k=1}^n \frac{c_k}{s - z_k},$$

where $C = r_n(\infty)$ and c_k is the residue of r_n at z_k . Then, assuming all the poles are enclosed by Γ , residue calculus converts (2.6) to

$$(2.8) \quad I_n = \sum_{k=1}^n c_k f(z_k).$$

This is our quadrature approximation to the integral I . If

$$(2.9) \quad \|\mathcal{C} - r_n\|_{\Gamma} \leq \varepsilon,$$

where $\|\cdot\|_{\Gamma}$ is the ∞ -norm on Γ , then by (2.5) and (2.6),

$$(2.10) \quad |I - I_n| \leq \frac{\varepsilon}{2\pi} |\Gamma| \|f\|_{\Gamma},$$

where $|\Gamma|$ is the arc length of Γ . If $|\Gamma|$ is large or infinite, it is often possible to remove this factor while replacing $\|\mathcal{C} - r_n\|_{\Gamma}$ or $\|f\|_{\Gamma}$ by the corresponding 1-norm.

The same reasoning just outlined also applies if γ is a closed Jordan contour, that is, a complex homeomorphism of the unit circle. All that changes now is that for Γ to “enclose” γ , it should consist of two Jordan contours, one inside γ and the other outside, as sketched on the right in Figure 1.

3. Application 1: Gauss–Legendre quadrature. The most basic quadrature problem is integration of a function f over the interval $\gamma = [-1, 1]$ with weight function $w(z) = 1$:

$$(3.1) \quad I = \int_{-1}^1 f(z) dz.$$

This is the original setting of Gauss quadrature, which is also called Gauss–Legendre quadrature to distinguish it from cases with non-constant weight functions (sections 5 and 6). Gauss derived his method by rational approximation of the Cauchy transform (2.4) of $w(z) = 1$ on $[-1, 1]$, which is $\mathcal{C}(s) = \log((s + 1)/(s - 1))$ [18, 19]. The only difference from the mathematics of the last section is that he used a Padé approximation at $s = \infty$ rather than an approximation over a contour Γ . This was before Cauchy integrals and long before Padé, so Gauss’s formulation, emphasizing continued fractions and hypergeometric series, is quite different from ours.

To illustrate the derivation of essentially the same quadrature formulas via rational approximation on a contour Γ , consider the test integrand $f(z) = 1/(1 + 20z^2)$,

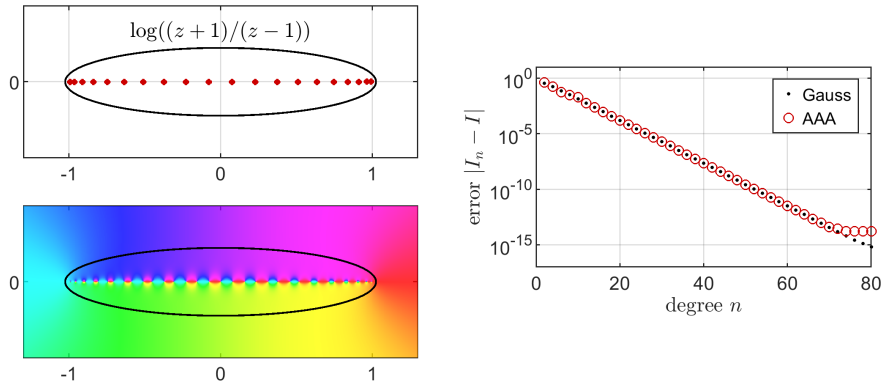


FIG. 2. Quadrature by AAA rational approximation of $C(s) = \log((z+1)/(z-1))$ on the Bernstein ellipse passing through the singularities at $\pm i/\sqrt{20}$ of the test integrand $f(z) = 1/(1+20z^2)$ on $[-1, 1]$. The upper-left image shows AAA poles for degree $n = 20$, close to the Gauss quadrature nodes of the same degree, and the lower-left image is a phase portrait of the AAA approximation $r_{20}(z)$ (red for positive real, cyan for negative real). The right image shows convergence for this integrand as a function of degree n .

which is analytic in the complex z -plane except at $z = \pm i/\sqrt{20}$. Motivated by standard results in approximation and quadrature, let us design a quadrature rule for functions analytic inside the Bernstein ellipse Γ (ellipse with foci ± 1) passing through these two points [54]. In the standard notation, this is the ellipse with parameter $\rho = 1/\sqrt{20} + \sqrt{21}/20 \approx 1.248$ (sum of semiminor and semimajor axis lengths). For AAA approximation, the degree n can be prescribed, or a tolerance for (2.9) can be specified so that n is determined adaptively. Here we compute an approximation $r_n(s) \approx \mathcal{C}(s)$ of degree $n = 20$ in about 0.05 s on a laptop with the code

```
rho = 1/sqrt(20) + sqrt(21/20);
c = rho*exp(2i*pi*(1:200)'/200);
Z = (c+1./c)/2;
F = log((Z+1)./(Z-1));
[r,pol,res] = aaa(F,Z,'degree',20,'sign',1);
```

(The 'sign' flag is discussed in section 8. As for the use of 200 sample points, the discretization details in these computations are usually not important, and one can bypass them by using the alternative continuum AAA algorithm [12, 14].) The three outputs from `aaa` are `r`, a function handle for the rational approximation, and `pol` and `res`, n -vectors of its poles and corresponding residues. Figure 2 shows that the poles look like Gauss quadrature points, and one can check that the weights are also close to Gauss weights. Following (2.8), a quadrature result can be obtained with

```
f = @(z) 1./(1+20*z.^2);
In = res.*f(pol)
```

and this gives $In \approx 0.603943 - 0.00000002i$, matching the exact value $I \approx 0.604100$ with an error of $1.6 \cdot 10^{-4}$.

In this and other experiments of this paper, the nodes and weights and computed integrals are all slightly complex even when one would expect them to be real. This is because the Chebfun implementation of AAA does not enforce real symmetry, although this can be fixed, as is done in some other implementations such as the `rational` code in the MathWorks RF Toolbox [41]. With such an adjustment, real

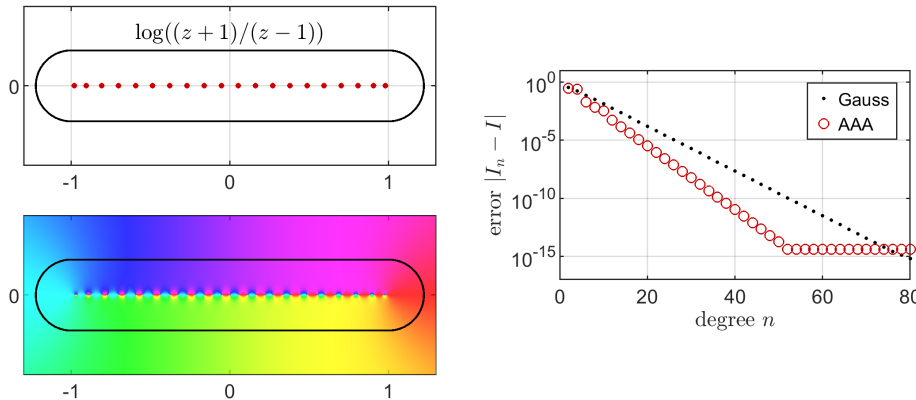


FIG. 3. Variant of Figure 2 in which $\log((z+1)/(z-1))$ is approximated on an ε -neighborhood of $[-1, 1]$ rather than a Bernstein ellipse. For the same test integrand as before, the convergence is now faster by a factor of about $\pi/2$, and the quadrature nodes are more evenly spaced.

symmetric problems give exactly real results.

The phase portrait in Figure 2 shows a clear approximation to the branch cut of $\log((z+1)/(z-1))$ along $[-1, 1]$, and the plot on the right shows that the convergence as a function of n closely matches that of Gauss quadrature. Here as in our later plots, convergence eventually stagnates for reasons related to rounding errors, which we do not attempt to analyze.

For a variant problem that Carl Gauss could not have handled, we start from the observation that although Gauss quadrature is commonly regarded as optimal, this is only true in specialized senses. Gauss quadrature is the unique n -point quadrature formula that integrates polynomials of degree $\leq 2n - 1$ exactly, and relatedly, it is optimal for integrands analytic in a Bernstein ellipse, which is a natural domain for polynomials. For integration of functions known to be analytic in domains other than ellipses, however, it is suboptimal [2, 55]. A more natural assumption to make about an integrand may sometimes be that it is analytic in an ε -neighborhood of $[-1, 1]$, and in [28], quadrature formulas were constructed for such classes based on conformal transplantation of a Bernstein ellipse. With rational approximation, we can get the same effect without the conformal mapping by changing the definition of the approximation set Z above from an ellipse to a stadium, like this:

```
ep = 1/sqrt(20);
Z = [-1i*ep+linspace(-1,1,100)'; 1+ep*exp(1i*pi*(-49:49)'/100)];
Z = [Z; -Z];
```

Figure 3 shows that for the same integrand $f(z) = 1/(1 + 20z^2)$ as before, the convergence is now faster by a factor of about $\pi/2$. Compare Figure 3.4 of [28] and Figure 4.1 of [55]. Perhaps more importantly, the quadrature nodes are more evenly spaced, a property that can be advantageous in time-stepping applications when there are CFL stability constraints [36]. The quadrature weights, which remain positive apart from complex perturbations, are also closer to uniform.¹

¹The reader may be puzzled how one can have nearly equispaced nodes without coming up against the Runge phenomenon of exponentially large weights with alternating signs. The explanation is that that is a phenomenon of polynomial interpolation, whereas here, the quadrature rule is implicitly

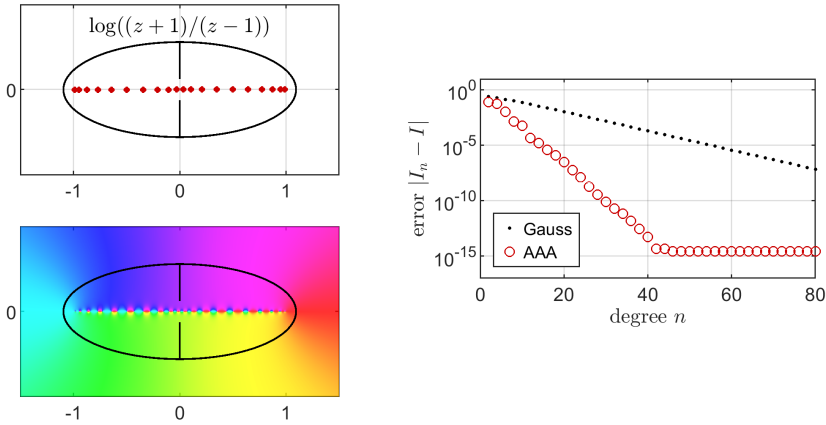


FIG. 4. Construction of a quadrature formula for an integrand with a conjugate pair of singularities near $[-1, 1]$, motivated by [52]. The test integrand is $1/(1 + 100z^2)$.

4. Application 2: Quadrature with nearby singularities. A theme of this article is that transplantation by conformal maps has been a tool often used for enhancing accuracy of integrals. A remarkable success in this direction was due to Wynn Tee in his construction of numerical methods for time-dependent blow-up and shock PDE problems [52]. (The second author was the junior partner in this work.) Using an adapted spectral spatial grid with as few as 56 points, Tee was able to resolve the solution to $u_t = u_{xx} + e^u$ on $[-1, 1]$ with homogeneous initial and boundary conditions up to a time within 10^{-8} of the blowup time of $t_c \approx 3.54466459$. Tee’s method can be described with reference to Figure 4. The difficulty in these problems is a pair of complex singularities approaching the real axis as $t \rightarrow t_c$, for singularities at distance ε would ordinarily require a grid of $O(\varepsilon^{-1})$ points. If the singularities are regarded as the ends of branch cut slits in the complex plane, however, he showed that a conformal transplantation can be used to send them far away, improving $O(\varepsilon^{-1})$ to $O(|\log \varepsilon|)$.

All this required careful analysis of conformal maps, but in the experiment shown in the figure, we have achieved the same effect (for quadrature rather than PDEs) by rational approximation. The same Cauchy transform $\mathcal{C}(s) = \log((z+1)/(z-1))$ as in the last section is now approximated on a Bernstein ellipse to which a conjugate pair of slits extending to $\pm 0.1i$ have been added. For the test integrand $f(z) = 1/(1 + 100z^2)$, whose singularities lie at the ends of the slits, one sees about a five-fold speedup over Gauss–Legendre quadrature. Closer singularities would amplify the effect. In Tee’s paper he estimates the singularity positions on the fly with Chebyshev–Padé approximation, which we would now propose to replace by AAA.

After the completion of [52], Hale and Tee generalized Tee’s method to problems with multiple conjugate pairs of singularities near the approximation interval [27]. Their generalization was again highly successful, but required expert Schwarz–Christoffel mapping. As a variant problem for this section, Figure 5 shows the same kind of improvement as in Figure 4 for a problem with several singularities. To highlight the flexibility of the method we have chosen a complex integrand whose singularities do not lie in conjugate pairs, namely $f(z) = \log([z - .01i]i) + \log([z - (.5 - .01i)]/i)$.

interpolating by rational functions [28].

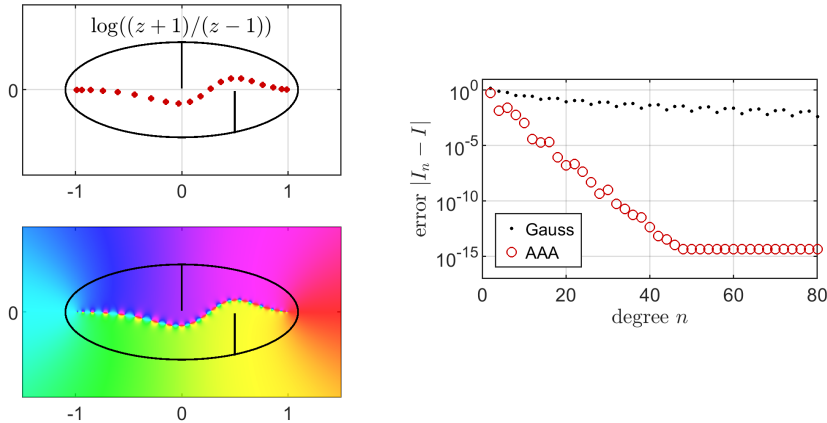


FIG. 5. Variant of Figure 4 inspired by [27] in which there may be several singularities near $[-1, 1]$, and not just conjugate pairs. The test integrand is $\log([z - .01i]/i) + \log([z - (.5 - .01i)]/i)$.

The snaky curve in the figure emphasizes the fact that in general, rational approximation chooses the contour as well as the nodes and weights. The examples of Figures 8, 9, 10, 11, 14, 16, and 17 are also notably of this kind. Indeed, near-optimal rational approximations are always choosing a near-optimal contour, and this merely fails to be apparent when the contour is simply a real interval for reasons of symmetry.

5. Application 3: Singular integrals. The method of section 2 is straightforward to adapt to a variety of challenging (and interesting!) non-constant weight functions $w(z)$ in (2.1). The new ingredient is that we need samples from the Cauchy transform of $w(z)$ to feed into AAA. In some special cases, just as for $w(z) = 1$ in the last two sections, the Cauchy transform can be determined analytically. In practice, it is convenient to evaluate it numerically on the contour Γ using an adaptive quadrature rule. In this and the next section we demonstrate this approach in two settings: first weakly singular integrals, then highly oscillatory ones.

For the first example, suppose $w(z)$ in (2.1) is integrable but not necessarily smooth or bounded. Numerical methods are often based on adaptive node refinement, analytic expansions, domain mapping, or hybrid schemes that combine these elements (for example, see “quadrature by expansion” [35] and references therein). Adaptive refinement may evaluate $f(z)$ many times, while analytic expansions and domain mapping techniques, for maximal efficacy, are derived on a case-by-case basis for different classes of weight functions. However, rational approximation offers the alternative of easy construction of Gauss-like formulas for arbitrary weights. To illustrate, consider the asymmetric Jacobi weight $w(z) = (1+z)^{3/2}(1-z)^{-1/2}$. This weight has algebraic singularities at both endpoints and blows up at the right endpoint. To obtain a quadrature rule with AAA, we compute samples of $\mathcal{C}(s)$ along the Bernstein ellipse of section 3 with Gauss–Kronrod quadrature as implemented in `quadgk` in MATLAB:

```
rho = 1/sqrt(20) + sqrt(21/20);
c = rho*exp(2i*pi*(1:400)/400);
Z = (c+1./c)/2;
w = sqrt(1+z).^3./sqrt(1-z);
F = @(z) arrayfun(@(zz) quadgk(@(z) w(z)./(zz-z),-1,1), z);
[r,pol,res] = aaa(F,Z,'degree',20,'sign',1);
```

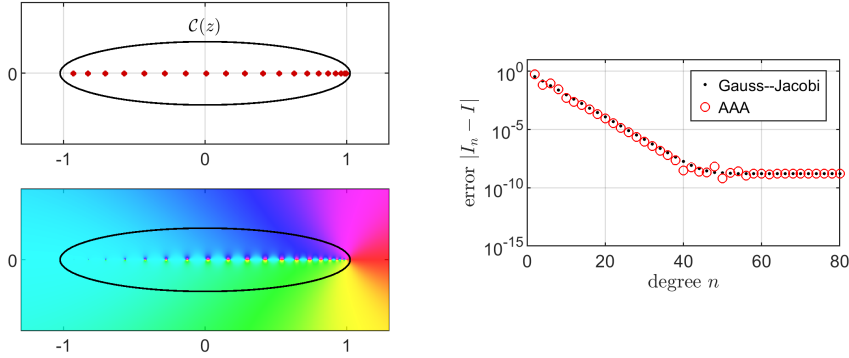


FIG. 6. AAA quadrature for the singular Jacobi weight function $w(z) = (1+z)^{3/2}(1-z)^{-1/2}$. The AAA poles cluster asymmetrically to capture the blow-up at $x = 1$.

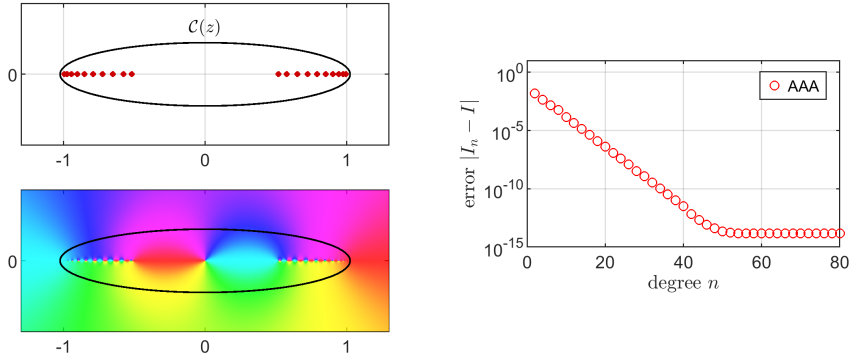


FIG. 7. AAA quadrature for the weight function (5.1). Poles appear only in the portions of $[-1, 1]$ where $w(z)$ is nonzero.

For higher-degree rules, one should adjust the default tolerances in `quadgk` to sample $\mathcal{C}(s)$ with sufficient accuracy. For this section, we set both 'AbsTol' and 'RelTol' to 10^{-13} . The left panel of Figure 6 displays the quadrature nodes (poles of $r_n(s) \approx \mathcal{C}(s)$) along with the phase portrait of r_n . The quadrature nodes cluster asymmetrically toward the right endpoint to capture the blow-up of $w(z)$ there, and the phase portrait makes it clear that that is where most of the action is. The Gauss–Jacobi nodes and weights associated with this weight function exhibit similar behavior (not shown). The right panel compares the convergence of AAA quadrature, for the same function $f(z)$ as in section 3, with that of the Gauss–Jacobi quadrature rule computed with `jacpts` in Chebfun. Clearly rational approximation has discovered rules that are essentially as effective as Gauss quadrature.

Our variant for this section concerns the non-classical weight function on $[-1, 1]$ defined by

$$(5.1) \quad w(z) = \begin{cases} \sqrt{1-z^2} & 0.5 \leq |z| \leq 1, \\ 0 & \text{otherwise.} \end{cases}$$

This weight function is supported on the disjoint intervals $[-1, -0.5]$ and $[0.5, 1]$ and

is not differentiable at any of the endpoints. Weight functions supported on disjoint intervals present a common challenge in the computation of response integrals in quantum chemistry and materials science, where points of non-differentiability at “band edges” or in the “bulk bands” are often associated with fascinating physical phenomena. High-order quadrature schemes must take care to resolve such singularities, which can degrade the convergence of popular “out-of-the-box” methods like the Kernel Polynomial Method (KPM) [50, 62].

AAA generates a new quadrature rule for the non-classical weight function with a single modification to the code above, namely, defining the new weight function. Figure 7 is the analogue of Figure 6 for the new AAA quadrature rule, and one can see that the quadrature nodes are confined to the support of the weight function. For this example, one could also design a specialized rule by partitioning the integration domain into $[-1, -0.5]$ and $[0.5, 1]$ and applying different Gauss–Jacobi rules on each subdomain. However, this strategy requires detailed knowledge of the location and type of each singularity. The AAA approach achieves similar performance while only requiring evaluation of the weight function on $[-1, 1]$.

6. Application 4: Oscillatory integrals. For our next application, suppose we want to compute an *oscillatory* integral of the form

$$(6.1) \quad I = \int_{-1}^1 f(z) \exp(i\omega g(z)) dz,$$

where $g(z)$ is a smooth *phase function* and ω is a real frequency. Such oscillatory integrals arise in scattering problems and related applications in, e.g., imaging. Traditional Gauss quadratures require many samples of $f(z)$ when ω is large, as they must satisfy the Nyquist sampling criterion associated with polynomial interpolation of the integrand. More efficient methods, which improve as ω increases, rely on specialized asymptotic expansions that exploit oscillation and cancellation in the integrand [11, 16, 37]. When $g(z)$ is analytic, the key ideas are those of stationary phase, to identify points of dominant contribution, and steepest descent, to identify paths in the complex plane along which the integrand decays exponentially. By deforming the contour off of $[-1, 1]$ along paths of steepest descent through points of stationary phase, one can truncate and apply Gauss quadrature on the deformed integral to derive methods that are convergent and of optimal order as $\omega \rightarrow \infty$ [10, 31].

Remarkably, the AAA approximation to the Cauchy transform of the weight function $w(z) = \exp(i\omega g(z))$ appears to generate quadrature rules of similar structure and similar efficiency. To illustrate, fix $\omega = 25\pi \approx 78.53$ and consider the simplest phase function, $g(z) = z$, corresponding to a band-limited Fourier transform. Since $g'(z) = 1$ is non-vanishing, there are no stationary points, and the dominant contribution to I comes from the endpoints. The classical “two-point” quadratures associated with highly oscillatory integrals approximate I with a weighted combination of f and its derivatives evaluated at the endpoints. For a fresh account with modern developments, see [32].

Now, as in the previous section, we compute the Cauchy transform of $w(z) = \exp(25\pi iz)$ on a Bernstein ellipse with $\rho = 2$ using `quadgk`. The samples of the Cauchy transform are fed to AAA, which generates a rational approximation of user-specified degree, whose poles and residues become the quadrature nodes and weights. Figure 8 shows that these quadrature nodes cluster densely at the endpoints of the interval. Moreover, they lie along nearly vertical arcs in the upper half-plane, with a slight inclination away from the ellipse. Further experiments (not shown) reveal that

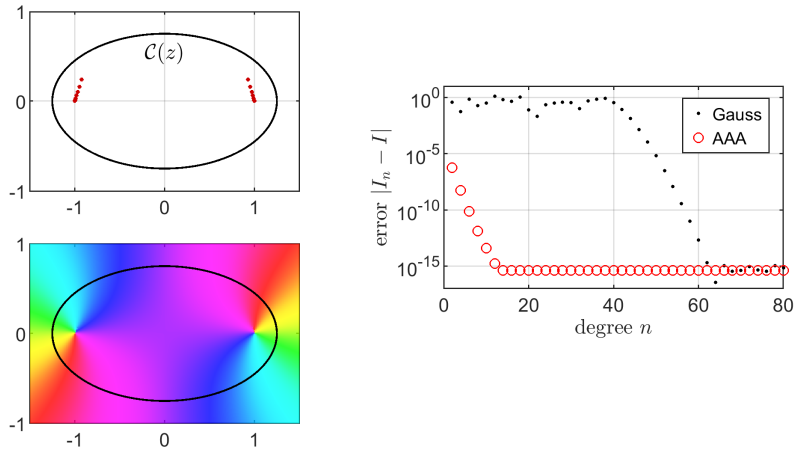


FIG. 8. AAA quadrature for the oscillatory integral in (6.1) with $\omega = 25\pi$ and $g(z) = z$. The quadrature nodes cluster near the endpoints along arcs that are close to paths of steepest descent. The right panel shows convergence for $f(z) = 1/(1 + z^2/4)$ as the degree of the quadrature rule is refined and compares with Gauss–Legendre quadrature.

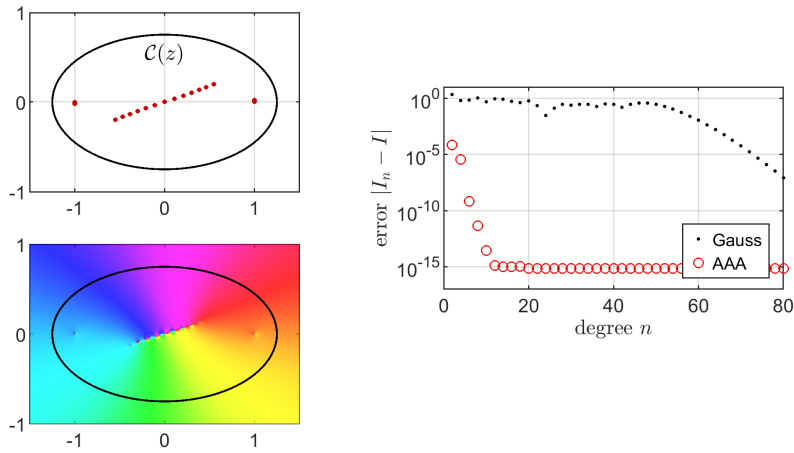


FIG. 9. Same as in Figure 8 but for the weight function $g(z) = z^4$.

when the Cauchy transform is sampled on a smaller Bernstein ellipse, the nodes crowd inward as if confined to the interior of the ellipse. When the ellipse is made larger, the nodes tend toward vertical lines in the upper half-plane—the paths of steepest descent for this Fourier integral.

For the variant, we consider the phase function $g(z) = z^4$, which has a stationary point of order 3 at $z = 0$. The associated path of steepest descent slices through the origin in the complex plane at an angle of $\pi/8$. The quadrature nodes computed by AAA again cluster at the endpoints, but now some of them distribute themselves evenly along an arc close to the path of steepest descent through $z = 0$. When the Cauchy transform is sampled on a smaller Bernstein ellipse (not shown), the nodes distribute themselves along an arc that is close to the path of steepest descent near the real line but curves away to fit within the ellipse off of the real line.

7. Application 5: Hankel contours for inverse Laplace transforms. John Butcher in the 1950s and Alan Talbot in the 1970s introduced the powerful technique of computing inverse Laplace transforms via discretizations of integrals over so-called *Hankel contours*,

$$(7.1) \quad I = \int_{\gamma} e^z f(z) dz \approx \sum_{k=1}^n c_k f(z_k).$$

A Hankel contour γ is an infinite arc in the complex plane wrapping around $(-\infty, 0]$ from $-\infty - 0i$ to $-\infty + 0i$ (and thus not precisely a homeomorphism of $[-1, 1]$). Here f is a function analytic in the simplest cases in $\mathbb{C} \setminus (-\infty, 0]$ which may be a scalar for applications to special functions or a large-dimensional matrix function for applications in computational science. Many researchers have worked with such techniques including Gallopoulos, Gavrilyuk, Gil, López-Fernández, Lubich, Luke, Makarov, McLean, Palencia, Schädle, Sheen, Sloan, Saad, Schmelzer, Temme, Thomée, and Trefethen, and the one who has investigated them most systematically is Weideman [58, 61]. See these papers and [57] for technical details and references.

To address (7.1) by rational approximation, we interpret e^z as a weight function on some Hankel contour; exactly which one doesn't matter. Since e^z is analytic, it follows from (2.4) that the Cauchy transform $\mathcal{C}(s)$ is e^s itself. The contour γ is deformed inward to $\Gamma = (-\infty, 0]$ (traversed from left to right along the bottom and then right to left along the top), and then in principle Γ should also include an outer boundary on which the value to be matched will be 0. However, this part of Γ does not need to be considered explicitly, as a rational approximation to e^z on $(-\infty, 0]$ will necessarily be ≈ 0 for $z \rightarrow \infty$. We can compute one with the code

```
Z = -logspace(-3,4,300)';
F = exp(Z);
[r,pol,res] = aaa(F,Z,'degree',14);
```

The degree 14 is fixed as the highest possible before reaching machine precision [54, chap. 20]. Figure 10 shows the very satisfactory result, with poles closely matching those in the papers cited above. A numerical calculation based on another integrand with integral 1,

```
f = @(z) -exp(1)/(1+z);
In = res.*f(pol)
```

gives the result $0.99999999999937 + 0.00000000000003i$ with error $6.3 \cdot 10^{-13}$. The convergence as a function of $n \rightarrow \infty$ closely tracks the optimal rate $(9.28903\dots)^{-n}$ [54, Thm. 25.2].

The elegant curve of poles on the left in Figure 10 echoes similar images to be found in Figures 3.1–3.3 and 4.3 of [58], where quadrature formulas are compared based on parabolic, hyperbolic, and cotangent (“Talbot”) contours as well as true best approximations of e^z on $(-\infty, 0]$. In the first three cases, exponential convergence rates on the orders of 2.85^{-n} , 3.20^{-n} , and 3.89^{-n} are obtained, whereas as we see in Figure 10, rational approximation gives the optimal rate of about 9.29^{-n} . This approximate doubling of the convergence rate, which we think of as the “Gauss quadrature factor of 2,” arises in many contexts of rational approximation in the difference between estimates obtained from potential theory arguments assuming $n + 1$ interpolation points of a rational approximation and the improved estimates, related to orthogonality, that come when there are $2n + 1$ interpolation points. See the end of [56] for a brief discussion and [47] for theorems.

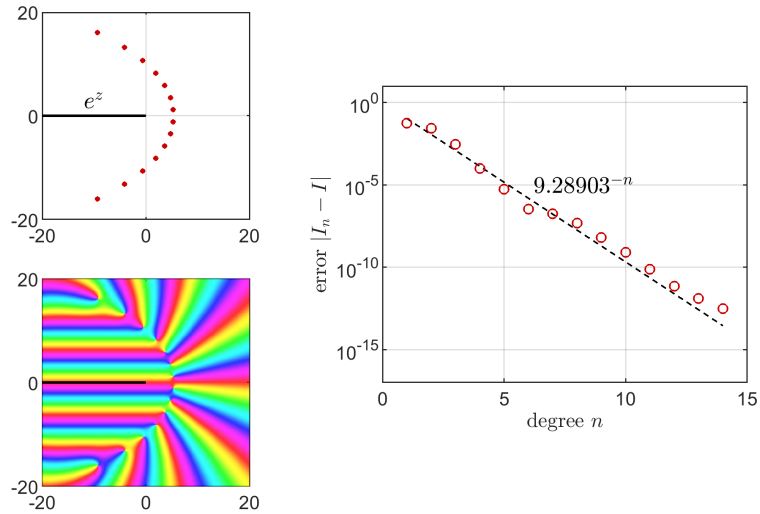


FIG. 10. Evaluation of the inverse Laplace transform by rational approximation following Butcher, Talbot, and many later authors. On the left, quadrature poles with $n = 14$, giving 12-digit accuracy for a test problem based on just 7 matrix solves (if real symmetry is exploited). The stripes in the phase portrait match those of e^z to the left of the curve of poles. On the right, convergence as a function of n , matching the optimal rate for best approximation.

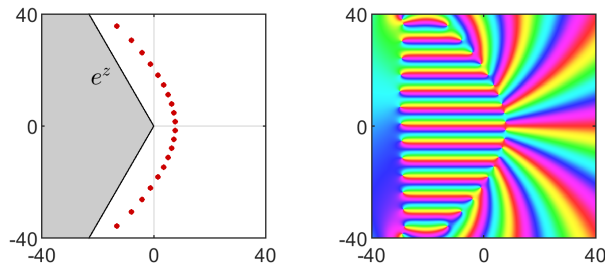


FIG. 11. Variant problem for a sectorial operator as in [38]. The reason the stripes terminate at around real part -35 is that e^{-35} is on the order of the accuracy of this approximant, close to machine precision.

Our variant problem for this section concerns a setting in which it is supposed that the function f , which may be derived from a matrix or operator, is *sectorial*, meaning that it is analytic and satisfies a growth condition outside a wedge in the left half-plane [38, 61]. A small change in the definition of the approximation domain,

$$\begin{aligned} Z &= -\text{logspace}(-3, 4, 300)'; \\ Z &= [\text{flipud}(Z)/\exp(.333i*\pi); Z*\exp(.333i*\pi)]; \end{aligned}$$

gives the images of Figure 11, now with the degree increased from $n = 14$ to $n = 20$ since the problem is slightly harder.

8. AAA approximation of sign functions. The last five sections could have been written five years ago, based on the AAA and AAA-Lawson algorithms of [42] and [43]. In the next two sections we will turn to examples involving approximation on two disjoint contours (see the right image of Figure 1), where a rational approximation is needed to a function with two branches, and here, these original algorithms proved

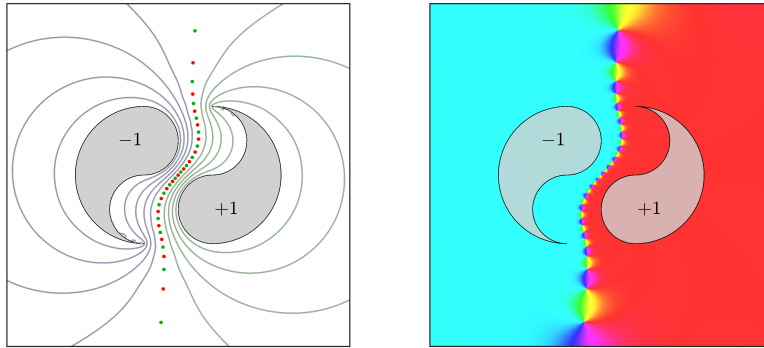


FIG. 12. Degree 20 rational approximation $r(z)$ of a sign function on a two-component yin-yang domain in the complex plane. On the left, the domain is shown together with poles (red) and zeros (green) of the rational approximation, defining an approximate branch cut, as well as error contours $|r(z) - (\pm 1)| = 10^{-1}, \dots, 10^{-4}$. On the right, a phase portrait of r .

unreliable. However, modifications were introduced in 2024 that make problems of this kind tractable too [59]. These variants are invoked by specifying the 'sign' and/or 'damping' options in calls to `aaa`. The first of these adjustments bases the AAA choice of a barycentric weight vector on a weighted blend of all the singular vectors of a Loewner matrix rather than just one, and the second introduces a damping factor in the update formula of the AAA-Lawson iteration. We will not discuss the details here, as they are treated in [59] and the topic of this paper is the link from rational approximation to quadrature, not the mechanics of rational approximation.

To illustrate the new capabilities, here is an example adapted from [59] of AAA computation of an approximate sign function. Suppose it is desired to find a rational function r_n of degree $n = 20$ that comes as close as possible to taking the values -1 and $+1$ on the two components of the yin-yang domain of Figure 12. This is an example of “Zolotarev’s 4th problem,” also known as the Zolotarev sign problem [33, 59]. We discretize the domain by 300 points on the boundary of each component.

```
c = exp(1i*pi*(1:100)'/100)/1i;
yin = [-c; conj(1i*c)/2i-.5i; c/2+.5i] - 1/2;
yang = -yin;
Z = [yin; yang];
```

No single analytic function can match the values -1 and 1 exactly; there must be a branch cut. Near-best rational approximations mimic this behavior by forming approximate branch cuts out of strings of poles and zeros. The rational approximation is computed in about 0.7 s on a laptop by these commands:

```
F = [-ones(size(yin)); ones(size(yang))];
[r,pol,res,zer] = aaa(F,Z,'degree',20,'sign',1);
plot(yin,'-k'), hold on, plot(yang,'-k')
plot(zer,'.g'); plot(pol,'.r');
```

The error contours in the figure can be understood at least approximately—and exactly, in the limit $n \rightarrow \infty$ —by methods of potential theory [56]. The potential function in question is generated by positive and negative charges on the two components distributed in a minimal-energy configuration.

The example of Figure 12 can be regarded as a prototype of the kind of rational approximation needed for applications involving Cauchy integrals over closed contours γ that separate \mathbb{C} into an interior and an exterior region.

9. Application 6: Trapezoidal rule on a circle. Here and in the next section we derive quadrature formulas for problems with closed contours, beginning with the simplest case of an integral around a circle. If g is an analytic function on the unit circle $\gamma = S = \{z \in \mathbb{C} : |z| = 1\}$, it has a Laurent series

$$(9.1) \quad g(z) = \sum_{k=-\infty}^{\infty} c_k z^k, \quad c_k = \frac{1}{2\pi i} \oint_S z^{-1-k} g(z) dz.$$

Since the work of Lyness in the 1960s, it has been recognized that integrals like this can be accurately evaluated by the trapezoidal rule with sample points at the n th roots of unity $\{z_k\}$ for some n [39, 40, 57]. For any f analytic on S ,

$$(9.2) \quad \frac{1}{2\pi i} \oint_S f(z) dz \approx \sum_{k=1}^n \frac{z_k}{n} f(z_k).$$

Indeed, this is the standard method for computing Taylor and Laurent coefficients, with adjustments to optimize the radius of the circle of evaluation depending on f [4, 17]. For a review of the history of this technique with many more references, see [1]. Applications in numerical linear algebra include many of those referenced in the opening paragraph.

For this problem the weight function is $w(z) = 1/(2\pi i)$ and the Cauchy transform is

$$(9.3) \quad \mathcal{C}(s) = \begin{cases} 1 & s \text{ interior to } \gamma, \\ 0 & s \text{ exterior to } \gamma. \end{cases}$$

Thus $\mathcal{C}(s)$ has a jump of the simplest kind across γ . Let us suppose that f is analytic in the annulus $\Omega = \{z \in \mathbb{C} : r^{-1} \leq |z| \leq r\}$ for some $r > 1$. (The results will depend little on the choice of r .) As our enclosing contour Γ of the kind shown on the right in Figure 1, we take

$$(9.4) \quad \Gamma = r^{-1}S \cup rS$$

with positive orientation on rS and negative on $r^{-1}S$. We now find a degree n rational function r_n that approximates \mathcal{C} on Γ as in (2.9). The following code requests an approximation with accuracy 10^{-8} :

```
S = exp(2i*pi*(1:100)'/100);
Z = [2*S; 0.5*S];
F = [zeros(size(S)); -ones(size(S))];
[r,pol,res] = aaa(F,Z,'tol',1e-8,'sign',1,'lawson',20);
```

The near-best approximation obtained has degree $n = 31$, with 31 poles ranging in modulus from 0.968 to 0.970, plotted on the left in Figure 13. The phase portrait of $r(z) + \frac{1}{2}$, with the constant $\frac{1}{2}$ added to ensure a separation between values $r(z) \approx -1$ and $r(z) \approx 0$, shows bright cyan in the interior of the disk and bright red in the exterior. To check the accuracy of the approximation as a quadrature formula, we apply it to (9.2) with integrand $f(z) = -2\sqrt{z^2 - 1/4}$, which has a pair of branch

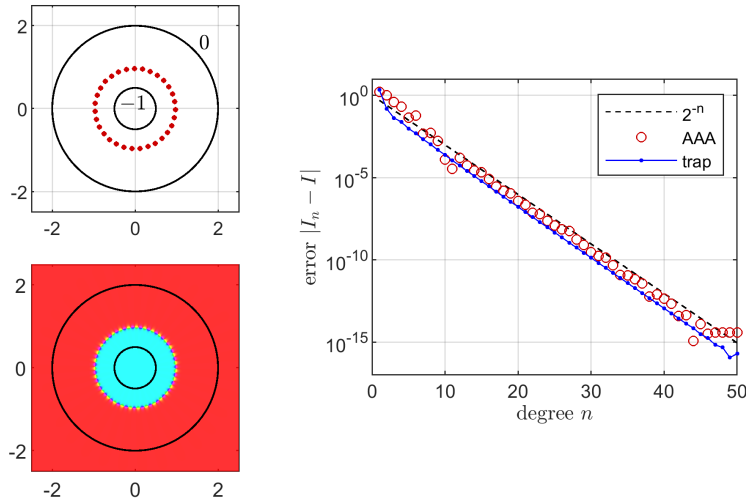


FIG. 13. On the left, quadrature nodes—poles of a degree $n = 31$ rational function—computed in about 0.05 s on a laptop by AAA rational approximation of a two-branch target function with accuracy specification 10^{-8} . The resulting approximate integral (9.2) has accuracy $2 \cdot 10^{-10}$, as compared with $7 \cdot 10^{-11}$ for the exact 31-point trapezoidal rule. The phase portrait now shows $r(z) + \frac{1}{2}$ to separate values ≈ -1 and ≈ 0 . On the right, errors as a function of n .

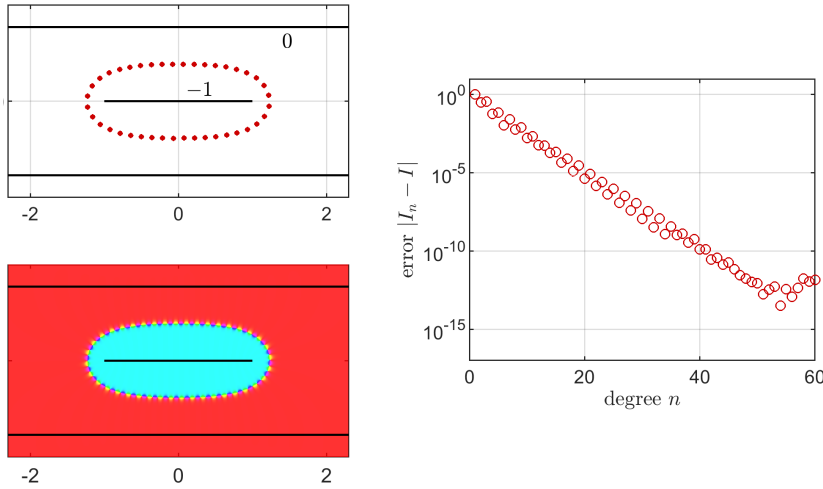


FIG. 14. Repetition of Figure 13 based on the assumption that f is analytic in the strip $-1 \leq \text{Im}z \leq 1$ minus the unit interval $[-1, 1]$.

points at $z = \pm 1/2$. The computed result I_n is $0.99999999901 + 0.00000000144i$, matching the correct value 1 with an error of about $2 \cdot 10^{-10}$. The exact 31-point trapezoidal rule of (9.2) would improve this just a little bit to $7 \cdot 10^{-11}$.

For the variant problem of this section, shown in Figure 14, we suppose that it is known that f is analytic not in a circular annulus but in the region of the strip $-1 \leq \text{Im}z \leq 1$ exterior to the unit interval $[-1, 1]$. One could derive a quadrature formula for this geometry analytically by conformal mapping, but this would take some work, and any modification of the geometry would require a new analysis. Instead we proceed numerically and change the discretization above to

```

segment = linspace(1,1,200)';
long = tan(pi*(-99:99)/200);
Z = [long+1i; long-1i; segment];
F = [zeros(size([long; long])); -ones(size(segment))];
[r,pol,res] = aaa(F,Z,'tol',1e-8,'sign',1,'lawson',20);

```

The approximation comes out with degree 40, and we test it on another function with integral 1, $f(z) = -\sqrt{(z-1)/(z+1)}$. The result is $0.999999999956 - 0.000000000024i$ with error $5.0 \cdot 10^{-11}$.

10. Application 7: Functions of matrices via Cauchy integrals. A function of a matrix or operator A can be defined by a Cauchy integral [29, 34],

$$(10.1) \quad f(A) = \frac{1}{2\pi i} \int_{\Gamma} f(z)(zI - A)^{-1} dz,$$

where Γ is a closed contour enclosing the spectrum of A and contained in the region of analyticity of f . This suggests the use of discretizations to approximate $f(A)b$ for a given vector b by a linear combination of vectors $(z_k I - A)^{-1}b$, where $\{z_k\}$ are quadrature nodes. For example, suppose A is a symmetric positive definite matrix with eigenvalues in $[m, M]$ for some $0 < m < M < \infty$, as suggested in the right image of Figure 15, and suppose f is a function like A^α or $\log(A)$ that is analytic in $\mathbb{C} \setminus (-\infty, 0]$. Then the trapezoidal rule with n equally spaced points could be applied over a circle passing through the point $z = m/2$, but the convergence as $n \rightarrow \infty$ would be very slow, requiring $O(M/m)$ linear solves for each reduction of the error by a constant factor. In the “three Nicks paper” [26], it was shown that this number can be improved enormously to $O(\log(M/m))$ by a conformal map involving Jacobi elliptic functions, as shown in the figure.² Now the mathematics is equivalent to the application of the trapezoidal rule on a circular annulus that is conformally equivalent to $\mathbb{C} \setminus \{[m, M] \cup (-\infty, 0]\}$. This corresponds to a fast-converging transplanted quadrature formula in unevenly spaced points in the z -plane.

To treat the problem by rational approximation instead of conformal mapping, we note that this is another case where the contour γ is flexible, to be determined, and the Cauchy transform will again be (9.3). Thus we can adjust the code segment of the last section to

```

segment = logspace(log10(1/8),0,100)';
negreal = 1 - 1./linspace(.005,1,100)';
Z = [negreal; segment];
F = [zeros(size(negreal)); -ones(size(segment))];
[r,pol,res] = aaa(F,Z,'degree',32,'sign',1,'lawson',0);

```

The poles shown on the left in Figure 16 are strikingly similar to those of Figure 15, even though neither a contour nor a node distribution has been fixed a priori. Choosing another integrand with integral exactly 1, $f(z) = (16/7)\sqrt{(z-1/8)/(z-1)}$, gives the result $1.000000000092 - 0.000000000000i$ with error magnitude $9.2 \cdot 10^{-11}$. This problem is more delicate than the last, and for clean results as a function of degree n , shown on the right in Figure 16, we modified the call to `aaa.m` to

```

[r,pol,res] = aaa(F,Z,'degree',n,'sign',1,'lawson',50,'damping',.5);

```

²Zolotarev was an expert in elliptic functions, and the mathematics here is very close to some of his work, though so far as we are aware, he did not make connections between rational approximation and quadrature.

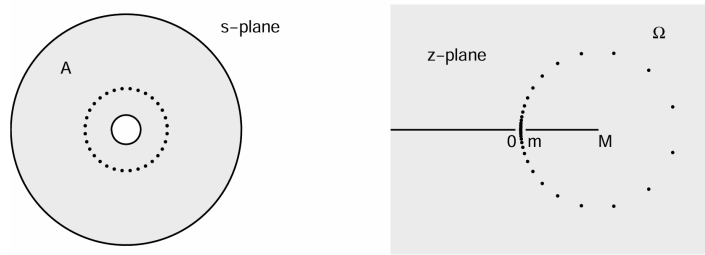


FIG. 15. A figure from [26] showing conformal transplantation of the 32-point equispaced trapezoidal rule in a circular annulus to a domain $\mathbb{C} \setminus \{[m, M] \cup (-\infty, 0]\}$ with $m = 1/8, M = 1$. This leads to fast evaluation of functions like A^α or $\log(A)$ if A is symmetric positive definite with spectrum contained in $[m, M]$.

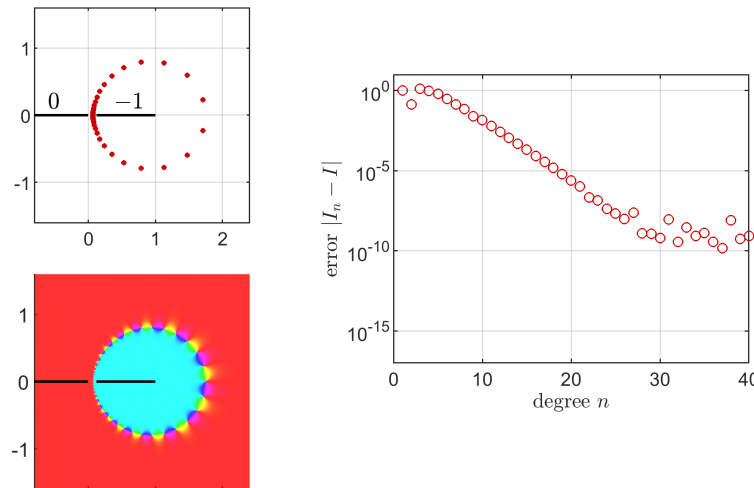


FIG. 16. Treatment of the same problem by rational approximation. On the left, quadrature poles with $n = 32$, giving 8-digit accuracy for a test problem. On the right, convergence for a test problem as a function of n .

Such adjustments reflect the fact that with the rational approximation algorithms of 2025, hand-tuning is often needed to get the best results. We hope that the situation will improve in the next few years as the algorithms mature.

The variant problem of this section was suggested to us by Maria López-Fernández of the University of Malaga. What if A is not symmetric but is known to have its spectrum in a given region of the right half-plane, like a rectangle? Figure 17 shows that the approximation r now has poles extending much further away from the origin, forming a bend of close to 90° near the spectrum.

11. Discussion. Nothing is entirely new in the field of quadrature, and the link with rational functions starts with Gauss in 1814 [18] and has been exploited in many ways since then. Most of this work has been algebraic, however, related to Padé approximations at ∞ and associated orthogonal polynomials. This paper has followed a more analytic approach based on numerical rational approximations made possible by the AAA algorithm. Here there is a smaller tradition, including the contributions

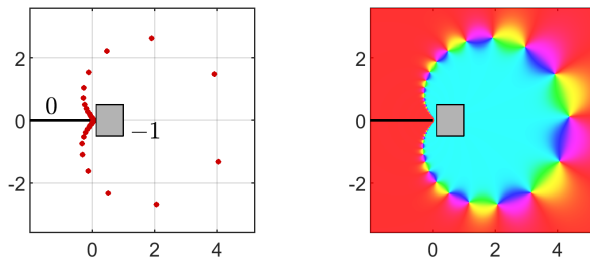


FIG. 17. A variant of Figure 16 in which the spectrum of A lies in a rectangle.

[51, 53, 58].

Whenever you see a string of quadrature nodes, you should consider it as a rational approximation to a branch cut. That is our conceptual message. Our practical message is that it is amazingly easy to compute near-optimal quadrature formulas by taking advantage of this connection. We make no claim that any of the particular techniques we have illustrated will immediately bring improvements in computational science, but we have outlined many possibilities and are confident that some of them will prove useful.

Jumps of complex functions across arcs arise in many contexts and are associated with notions including Cauchy/Stieltjes/Hilbert transforms, the Sokhotski–Plemelj formula, Wiener–Hopf factorization, the Dirichlet-to-Neumann map, and Riemann–Hilbert problems. The literature of such topics is enormous, and links could be found from this paper to most of it. Another topic in this space is that of *hyperfunctions*, which are generalized functions realized as (equivalence classes of) pairs of analytic functions on either side of an arc [22]. The present paper could be said to investigate quadrature formulas as rational hyperfunction approximations to Cauchy transforms. Perhaps this work can help encourage the growth of a numerical theory of hyperfunctions, which has been mostly a theoretical topic heretofore.

Theoretical questions lie around every corner. Exactly what are the links with potential theory? Does the phenomenon of “balayage” [23] relate interpolation points at ∞ , for example, to almost equally effective points along a Bernstein ellipse? Can backward error analysis confirm our experience that nodes and weights may be individually far from optimal yet still combine to give nearly optimal quadratures? Can one prove in some generality that best rational approximations match the convergence rates of Gauss quadrature rules? When can weights (= residues) be guaranteed to be positive, or at least uniformly summable as $n \rightarrow \infty$? These are just a few examples of many problems to be explored.

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