

Rational Approximation

Lloyd N. Trefethen *

July 19, 2024

Rational approximation is an old subject, but it has gone through a transformation in recent years with the appearance of a new algorithm that makes computing rational approximations easy. Indeed, many problems can now be solved to good accuracy in milliseconds on a laptop. This is the AAA algorithm, whose name derives from “adaptive Antoulas-Anderson” [NST18]. Curiously, the computation of polynomial approximations on domains other than intervals and disks, which is in principle a much easier problem but still becomes numerically intractable if a good basis is not available, has also been transformed recently by the introduction of the so-called Vandermonde-with-Arnoldi algorithm [BNT21].

The aim of this short story is not to describe these algorithms, which has been done elsewhere, but to show how beautifully they can reveal the power of rational functions and the mathematics of rational approximation. With the help of six figures all in the same format, we will illustrate what is sometimes called the Walsh/Gonchar theory of this subject. Details and references can be found in [LS06, NST18, Rak16, Tre23].

The setting is a function f defined on a compact, simply connected set K in the complex plane \mathbb{C} , and $\|\cdot\|$ is the ∞ -norm over K . (Simple connectivity doesn’t matter for the algorithm, but it makes this exposition simpler.) We are interested in best or near-best approximations to f by rational functions r of degree n (i.e., $r = p/q$ with polynomials p and q of degree n), and for comparison, by polynomials of

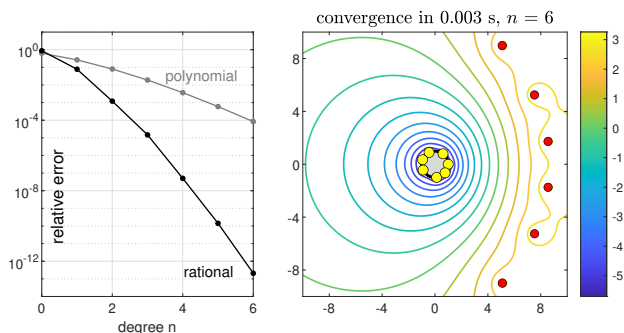


Figure 1: Entire function, $f(z) = \exp(z)$

degree n . The minimax errors can be written

$$E_n = \inf_p \|f - p\|, \quad E_{n,n} = \inf_r \|f - r\|.$$

First, consider the case where f is entire. Here it is known that both E_n and $E_{n,n}$ are guaranteed to decrease super-exponentially as $n \rightarrow \infty$, i.e., they are both $O(C^{-n})$ for any $C > 1$. Figure 1 illustrates this for approximation of $f(z) = e^z$ on the unit disk. On the left, we see convergence curves for AAA rational and Vandermonde-with-Arnoldi polynomial approximation, curving downward on this log scale. On the right, we see a portion of the complex plane with information about the final rational r approximation to accuracy 10^{-12} , of degree $n = 6$ in this case. The red dots mark the poles $\{\pi_k\}$ of r , $1 \leq k \leq n$. The yellow dots mark a set of interpolation points $\{z_k\}$ with $f(z_k) = r(z_k)$, $0 \leq k \leq n$, that are selected by AAA in the course of its computation. The AAA algorithm is a “greedy” iteration based on a barycentric representation of r with coefficients determined by a least-squares minimization [NST18]. There may

*Professor of Applied Mathematics in Residence, School of Engineering and Applied Sciences, Harvard University

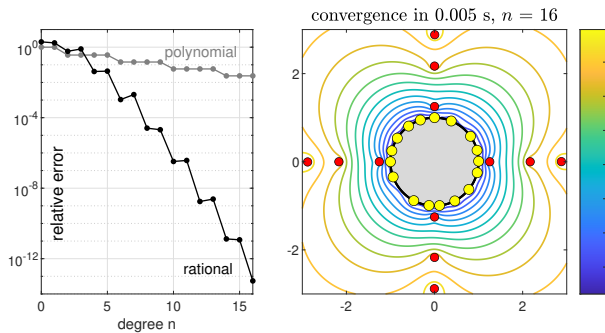


Figure 2: Meromorphic function, $f(z) = \tan(z^2)$

be other points besides $\{z_k\}$ where r also interpolates the data, but the plots just mark these $n+1$ “support points” explicitly selected step by step by AAA. (Because of the least-squares aspect of AAA, sample sets for $f(z)$ do not have to be determined carefully; it is usually enough to distribute a few hundred sample points with reasonable density along the boundary of the domain.) The contours in this and the other plots are potential curves associated with the poles and interpolation points, as we will explain at the end.

Next, suppose f is analytic on K but meromorphic in $\mathbb{C} \setminus K$, having one or more poles. Here rational approximations can “peel the poles off,” so the decay of $E_{n,n}$ is still superexponential. Polynomials, however, are limited to exponential convergence at a rate determined by the pole closest to K as measured by a conformal map of $\mathbb{C} \setminus K$ to the exterior of the unit disk [Tre24, Thm. 3]. Figure 2 illustrates all this for $f(z) = \tan(z^2)$ on the unit disk, with the rational curve again curving downward but the polynomial curve now straight. (Four poles are off-scale, and similarly there are 4, 1, 4, and 5 poles off-scale in Figures 3, 4, 5, and 6.)

Now suppose f has essential singularities outside K . You might expect this to slow down rational approximations fundamentally, but in fact, the convergence is still superexponential, as shown in Fig. 3 for $f(z) = \exp(\tan(z^2))$ on the unit disk. The contour plot looks much as in Fig. 2, but each of the inner four red dots is now a cluster of five poles, as illustrated in the inset.

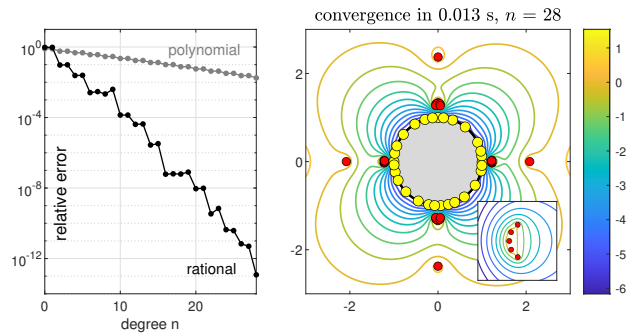


Figure 3: Function with essential singularities, $f(z) = \exp(\tan(z^2))$. Inset: zoom near $z = \sqrt{\pi/2}$

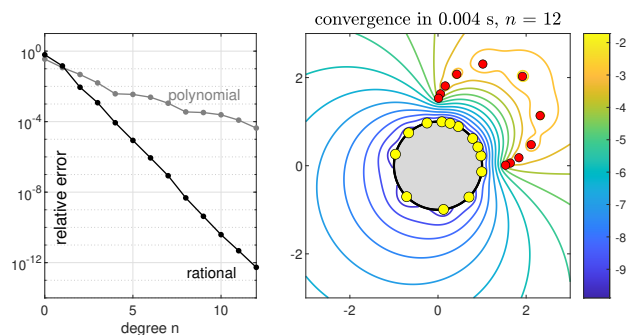


Figure 4: Function with branch points, $f(z) = \sqrt{(1.5-z)(1.5i-z)}$

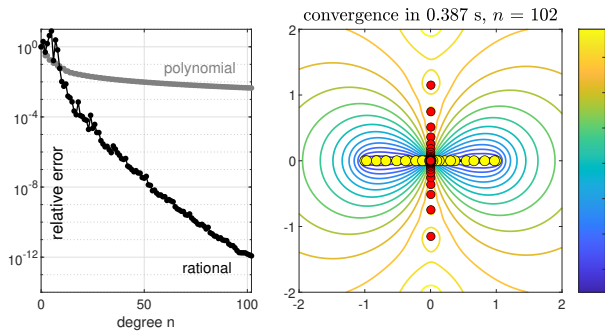


Figure 5: Function with singularity on the approximation domain, $f(z) = |z|$ on $[-1, 1]$

Branch points are a more serious obstacle to approximation, because they are not isolated singularities. If f has any branch points outside K , rational approximants always slow down to exponential convergence. Thus both rational functions and polynomials converge exponentially, but the rates may be very different. I like to think that the trouble with polynomials is that their poles are constrained to lie at ∞ , whereas rational functions can put poles wherever they are most useful. The poles of good rational approximations do their best to approximate branch cuts, lining up beautifully along certain curves investigated by Stahl [Sta97], as one sees in Fig. 4 for approximation on the unit disk of a function with square root singularities at $z = 1.5$ and $1.5i$.

Finally, there are two great cases where rational functions are far more efficient than polynomials. The well-known one, as discovered by Newman in 1964 [New64], is when f has branch point singularities on the boundary of K . Here, polynomials are stuck with algebraic convergence, whereas rational functions can achieve root-exponential convergence ($O(C^{-\sqrt{n}})$) by clustering poles exponentially near the singularities. Figure 5 shows Newman’s example of approximation of $f(z) = |z|$ on $[-1, 1]$. The rational approximations converge root-exponentially, whereas the polynomials do no better than $O(1/n)$.

The other case is not so well known but equally important. This is the situation of approximation on a nonconvex domain when the analytic continuation of f has a singularity in an “inlet”, as will be true

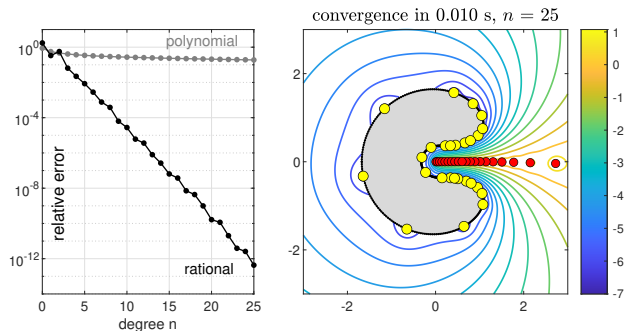


Figure 6: Function analytic in a nonconvex region, $f(z) = \sqrt{-z}$

in most applications. Here both polynomials and rational functions achieve exponential convergence, $\|f - r\| = O(C^{-n})$ for some $C > 1$, but for polynomials, C is exponentially close to 1 with respect to the length of the inlet [Tre24, sec. 7]. In the case shown in Fig. 6, involving a smooth domain K bent around a portion of the positive real axis, we would need to increase the degree of p asymptotically by about 500 for each additional digit of accuracy. In such cases, for practical purposes, polynomials effectively do not converge at all. The rational functions do fine by approximating a branch cut along $[0, \infty)$.

Now at last let us explain the contours in the figures, which show off the Walsh/Gonchar theory that leads to all of the results we have outlined. These contours are level curves of a potential function ϕ which we can interpret as generated by a positive point charge at each pole π_k and a negative point charge at each interpolation point z_k ,

$$\phi(z) = \prod_{k=0}^n (z - z_k) \bigg/ \prod_{k=1}^n (z - \pi_k). \quad (1)$$

This yields an error estimate for r by a Cauchy–Hermite contour integral exploited by Joseph Walsh beginning in the 1930s [Wal65, Thm. 8.2],

$$f(z) - r(z) = \frac{1}{2\pi i} \int_{\Gamma} \frac{\phi(z)}{\phi(t)} \frac{f(t)}{t - z} dt. \quad (2)$$

This identity holds for any contour Γ within which f and r are analytic, and good bounds come when the

pole and interpolation point distributions are close to equilibrium. Behavior as $n \rightarrow \infty$ was investigated by Gonchar and others beginning in the 1960s, and the best bounds come with Γ lying “as far from K as possible,” hugging Stahl’s optimal branch cuts. The AAA algorithm doesn’t know the Walsh/Gonchar theory, but its poles delineate the optimal branch cuts pretty well anyway.

Something remarkable emerges if one examines the numbers on the colorbars in our plots. These represent powers of 10, and what is striking is that the range of yellow to blue is typically around 7 orders of magnitude, not 12 or more as (2) would suggest for 12-digit accuracy. There is a factor of 2 in play here that is related to a certain orthogonality or approximate orthogonality along contours. Simply put, taking absolute values in eq. (2) gives a valid upper bound, but the actual error is often much smaller because of oscillation of the integrand, leading to cancellation of the integral to leading order. For many near-best approximations, $E_{n,n}$ is on the order of the square of what one would expect from (2). Rakhmanov speaks of the *Gonchar-Stahl ρ^2 theorem*, which details cases in which this squaring can be guaranteed. See [Rak16] and [Tre23, sec. 7.5].

The easy computations and plots of this review would not have been possible before about 2018. The implications of the AAA algorithm are very wide-ranging, making rational functions practical for numerical computation in a way they were not before. Exploring the possibilities is an active research area in numerical analysis.

References

- [BNT21] P. D. Brubeck, Y. Nakatsukasa, and L. N. Trefethen, *Vandermonde with Arnoldi*, SIAM Rev. **63** (2021), no. 2, 405–415. MR4253796
- [LS06] E. Levin and E. B. Saff, *Potential theoretic tools in polynomial and rational approximation*, Harmonic Analysis and Rational Approximation, 2006, pp. 71–94.
- [New64] D. J. Newman, *Rational approximation to $|x|$* , Michigan Math. J. **11** (1964), 11–14. MR1711113
- [NST18] Y. Nakatsukasa, O. Sète, and L. N. Trefethen, *The AAA algorithm for rational approximation*, SIAM J. Sci. Comput. **40** (2018), no. 3, A1494–A1522. MR3805855
- [Rak16] E. A. Rakhmanov, *The Gonchar-Stahl theorem and associated directions in the theory of rational approximations of analytic functions*, Sbornik: Mathematics **207** (2016), no. 9, 1236.
- [Sta97] H. Stahl, *The convergence of Padé approximants to functions with branch points*, J. Approx. Theory **91** (1997), no. 2, 139–204. MR1484040
- [Tre23] L. N. Trefethen, *Numerical analytic continuation*, Jpn. J. Ind. Appl. Math. **40** (2023), no. 3, 1587–1636. MR4644441
- [Tre24] ———, *Polynomial and rational convergence rates for Laplace problems on planar domains*, 2024. submitted.
- [Wal65] J. L. Walsh, *Interpolation and Approximation by Rational Functions in the Complex Domain*, 4th ed., American Mathematical Society, Providence, RI, 1965. MR218588