Low-rank approximations of the Cauchy kernel

Jonathan E. Moussa Molecular Sciences Software Institute, Blacksburg, VA

Abstract

This note compares two forms of low-rank approximation of the Cauchy kernel: interpolative decompositions and exponential sums. There is strong evidence that interpolative decompositions are optimal with respect to pointwise relative error and that exponential sums are asymptotically optimal as the number of exponentials increases.

1 Introduction

Here I consider the problem of low-rank approximation of the Cauchy kernel,

$$\frac{1}{x-y} \approx \sum_{i=1}^{n} f_i(x)g_i(y) \quad \text{for} \quad x \in \mathcal{X}, y \in \mathcal{Y},$$
 (1)

where X and Y are disjoint subsets of the complex plane. There are many ways to construct such approximations, depending on the choices of error metric, functional form, and approximation domain.

If the error metric is the pointwise relative error and the approximation domains X and Y are real, compact, and ordered (X > Y), then I have previously [3] shown that an interpolative decomposition,

$$I(x,y) = \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{x - y_i} \frac{\text{Res}(h, y_i) \text{Res}(1/h, x_j)}{y_i - x_j} \frac{1}{x_j - y}, \quad h(z) = \prod_{i=1}^{n} \frac{z - x_i}{z - y_i},$$
 (2)

is optimal if the only constraint on the form of f and g is that they are real-valued. An important property of this approximation form is that the pointwise relative error simplifies as

$$1 - (x - y)I(x, y) = h(x)/h(y). (3)$$

Thus, if the optimization is restricted to the interpolation form in Eq. (2), a variational upper bound on the error optimized over interpolation points is

$$\min_{f_i,g_i} \max_{x \in \mathcal{X}, y \in \mathcal{Y}} |1 - (x - y)I(x, y)| \le \min_{x_i,y_i} \max_{x \in \mathcal{X}, y \in \mathcal{Y}} |h(x)/h(y)|. \tag{4}$$

Showing equality of these formulas by proving the corresponding lower bound is a more complicated exercise of convex relaxations that I do not consider here. This minimax error is a specific instance of a Zolotarev number, more generally defined as

$$Z_n(X, \mathcal{Y}) = \inf_{h \in R_{n,n}} \frac{\sup_{x \in X} |h(x)|}{\inf_{y \in \mathcal{Y}} |h(y)|}$$
(5)

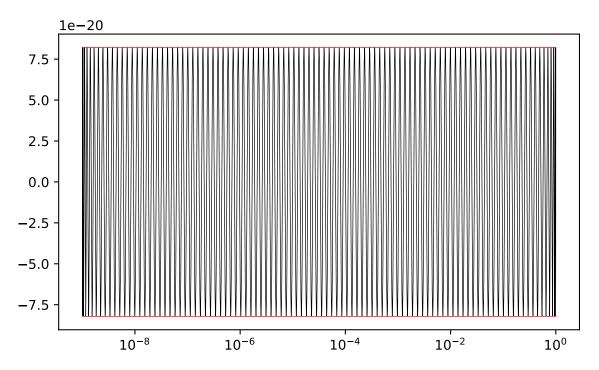


Figure 1: Rational function h that minimizes $Z_n(\lambda)$ for n = 200 and $\lambda = 10^{-9}$.

for a positive integer n, disjoint subsets X and Y of \mathbb{C} , and the set $R_{n,n}$ of rational functions with numerator and denominator of polynomial degree at most n. In this general setting, the infimum and supremum must be used because the minimum and maximum might not be well defined.

While Eq. (4) can be optimized numerically, there is an analytical solution for $X = [\lambda, 1]$ and $\mathcal{Y} = [-1, -\lambda]$ that was discovered by Zolotarev [4], which can be transformed to other disjoint pairs of real intervals using a Möbius transformation. I refer to this case specifically as $Z_n(\lambda) = Z_n([\lambda, 1], [-1, -\lambda])$. Its optimal interpolation points are

$$x_i = \operatorname{dn}\left(\frac{i-1/2}{n}K(1-\lambda^2), 1-\lambda^2\right) = -y_i,$$
 (6)

where K is the complete elliptic integral of the first kind and dn is a Jacobi elliptic function, both with the argument conventions used by the SciPy library in Python. For error estimation purposes, the value of $Z_n(\lambda)$ can be bounded as

$$Z_n(\lambda) \le 4 \exp\left(-n\frac{2\pi K(\lambda^2)}{K(1-\lambda^2)}\right) \le 4 \exp\left(-n\frac{\pi^2}{\log(4/\lambda)}\right). \tag{7}$$

SciPy can be used to evaluate the special functions in Eq. (6) unless λ is small enough that $1 - \lambda^2$ is rounded to 1 in double-precision arithmetic. In this extreme case, SciPy still provides direct access to K(1-x) for a user-specified value of x, but there is no equivalent feature for dn, so I use a custom implementation of dn with a similar interface. I show an extreme example in Fig. 1 to highlight numerical stability and the equioscillation behavior of the optimizing rational functions. Note that high relative accuracy requires h to be evaluated as the product shown in Eq. (2).

2 Exponential sums

Another popular approximation form for Eq. (1) is a sum of exponentials,

$$\frac{1}{x-y} \approx \sum_{i=1}^{n} w_i e^{-s_i(x-y)} \tag{8}$$

because it reduces to a simpler function approximation problem,

$$\frac{1}{z} \approx \sum_{i=1}^{n} w_i e^{-s_i z} \quad \text{for} \quad z \in \mathcal{Z} = \{x - y : x \in \mathcal{X}, y \in \mathcal{Y}\}. \tag{9}$$

There are several methods for constructing such approximations in the literature, by aligning the nodes of the residual error function between interpolative and sum-of-exponential forms [2] or as numerical integration quadrature [1]. Here I consider a more direct construction based on the interpolative decomposition. The basic idea is to start from a shifted Laplace transform decomposition of 1/z,

$$\frac{1}{z} = e^{s_{\min}z} \int_{s_{\min}}^{\infty} ds \, e^{-sz},\tag{10}$$

and a reconstruction of the exponential from Cauchy's integral formula with a contour along the imaginary axis that is closed over the positive reals,

$$e^{-sz} = \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} dt \frac{e^{-tz}}{t-s} \quad \text{for} \quad s, z > 0.$$
 (11)

By combining these two integral decompositions,

$$\frac{1}{z} = \frac{e^{s_{\min}z}}{2\pi i} \int_{s}^{\infty} ds \int_{-i\infty}^{i\infty} dt \frac{e^{-tz}}{t-s},\tag{12}$$

an exponential sum can be constructed directly from an interpolative decomposition of the Cauchy kernel.

The approximation domain of the Cauchy kernel in Eq. (12) is along both the imaginary axis with $t \in \mathbb{C}$ and along part of the real axis with s. It is necessary to restrict the domain of s, and I consider a domain $[-s_{\text{max}}, -s_{\text{min}}] \cup [s_{\text{min}}, s_{\text{max}}]$. I construct this approximation from Zolotarev's solution through a sequence of transformations. First, I use a Möbius transformation,

$$z' = s_{\min}^2 \frac{1 + \lambda'}{2\lambda'} \frac{z + \lambda'}{1 + z},\tag{13}$$

to transform $z \in [-1, -\lambda']$ to $z' \in (-\infty, 0]$ and $z \in [\lambda', 1]$ to $z' \in [s_{\min}^2, s_{\max}^2]$ for λ' satisfying

$$s_{\text{max}}^2 = s_{\text{min}}^2 \frac{(\lambda' + 1)^2}{4\lambda'}.$$
 (14)

Similarly, the Möbius transformation applies to the interpolation points to form the optimal interpolative decomposition of the Cauchy kernel on the transformed domain with transformed interpolation points x'_i and y'_i .

The second transformation step is less straightforward. I would like to apply a square root transformation to map the positive reals to the real axis and the negative reals to the imaginary axis, but the interpolative decomposition is not strictly invariant with respect to such a transformation. Instead, I consider a distinct interpolative decomposition with 2n pairs of interpolation points defined as $s_{\pm i} = \pm \sqrt{x_i'}$ and $t_{\pm i} = \pm \sqrt{y_i'}$ and labeled as

$$K(t,s) = \sum_{i} \sum_{j} \frac{1}{t - s_{i}} \frac{\text{Res}(k, s_{i}) \text{Res}(1/k, t_{j})}{s_{i} - t_{j}} \frac{1}{t_{j} - s}, \quad k(z) = \prod_{i} \frac{z - t_{i}}{z - s_{i}}.$$
 (15)

The same simplification of the pointwise relative error also applies to this case,

$$1 - (t - s)K(t, s) = k(t)/k(s). (16)$$

This error formula is then related to the original error formula as

$$\frac{k(t)}{k(s)} = \frac{h'(s^2)}{h'(t^2)}, \quad h'(z) = \prod_{i=1}^{n} \frac{z - x_i'}{z - y_i'},\tag{17}$$

so the pointwise relative error is still bounded by the same Zolotarev number, $Z_n(\lambda')$. However, the optimality of the interpolative decomposition is not preserved by this transformation - it is likely to still be within a constant multiplicative factor of optimal, but it is no longer strictly optimal.

To apply this interpolative decomposition of the Cauchy kernel to Eq. (12), I split the Laplace transform domain into $[s_{\min}, s_{\max}]$ and (s_{\max}, ∞) and use the decomposition only within the first domain to construct the exponential sum approximation

$$F(z) = \sum_{i}' w_i e^{(s_{\min} - s_i)z}, \quad w_i = \text{Res}(k, s_i) \left[\sum_{j} \frac{\text{Res}(1/k, t_j)}{s_i - t_j} \log \left(\frac{t_j - s_{\min}}{t_j - s_{\max}} \right) \right], \tag{18}$$

where the sum over i is restricted to positive s_i values because the negative poles do not contribute to the sum over residues in the positive real half plane when evaluating Cauchy's integral formula. The weights are all positive and can be further simplified as

$$W_i = \cdots$$
 (19)

The pointwise relative error in this approximation is

$$1 - zF(z) = e^{-(s_{\text{max}} - s_{\text{min}})z} + z \frac{e^{s_{\text{min}}z}}{2\pi i} \int_{s_{\text{min}}}^{s_{\text{max}}} ds \int_{-i\infty}^{i\infty} dt \frac{e^{-tz}}{t - s} \frac{k(t)}{k(s)},$$
 (20)

and the construction of error bounds requires an upper bound on this quantity. Although |k(t)/k(s)| on the integration domain is bounded by $Z_n(\lambda')$, the rest of the integrand is not absolutely integrable on this domain. It is possible to create an absolutely integrable domain by using a semicircle contour of a finite radius that encapsulates $[s_{\min}, s_{\max}]$, but the arc of the semicircle needs a separate bounding argument because |k(t)/k(s)| is not bounded by $Z_n(\lambda')$ on this new domain. If this alternate contour is effective, this approach could also utilize a more efficient domain transformation that maps $[-1, -\lambda']$ to the segment of imaginary axis along this contour rather than the complete imaginary axis. An error bound is needed before s_{\min} , s_{\max} , and possible the contour radius can be optimized to minimize the error of Eq. (9) on the approximation domain $[\lambda, 1]$. I am not sure that this approach to error analysis will work, but it is the most promising idea that I have right now.

Acknowledgement

The Molecular Sciences Software Institute is supported by grant CHE-2136142 from the National Science Foundation.

References

- [1] Gregory Beylkin and Lucas Monzón. "Approximation by exponential sums revisited". In: *Applied and Computational Harmonic Analysis* 28.2 (2010). Special Issue on Continuous Wavelet Transform in Memory of Jean Morlet, Part I, pp. 131–149. doi: https://doi.org/10.1016/j.acha.2009.08.011.
- [2] Dietrich Braess and Wolfgang Hackbusch. "Approximation of 1/x by exponential sums in [1, ∞)". In: *IMA Journal of Numerical Analysis* 25.4 (Oct. 2005), pp. 685–697. DOI: 10.1093/imanum/dri015.
- [3] Jonathan E. Moussa. *Minimax separation of the Cauchy kernel*. 2020. arXiv: 1909.06911 [math.NA].
- [4] John Todd. "Applications of Transformation Theory: A Legacy from Zolotarev (1847–1878)". In: *Approximation Theory and Spline Functions*. Ed. by S. P. Singh, J. W. H. Burry, and B. Watson. Dordrecht: Springer Netherlands, 1984, pp. 207–245. DOI: 10.1007/978-94-009-6466-2_11.