MINIMAX SEPARATION OF THE CAUCHY KERNEL

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Abstract. We prove and apply an optimal low-rank approximation of the Cauchy kernel over separated real domains. A skeleton decomposition is the minimum over real-valued functions of the maximum relative pointwise error. We establish a numerically stable form for the decomposition and demonstrate an example for which it is arbitrarily more accurate than singular value decompositions.

Key words. low-rank approximation, minimax approximation, Cauchy kernel, Cauchy matrix

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1. Introduction. Low-rank approximations of matrices and functions of two variables are useful primitives in numerical analysis [13]. For example, they are used in hierarchical matrices [8] and low-rank approximations of tensors and multivariate functions [7]. Truncated singular value decompositions (SVDs) are popular low-rank approximations because they are simple to compute and optimal with respect to the 2-norm. For a matrix $K \in \mathbb{R}^{m \times n}$ or an integral kernel $K : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$ between two Lebesgue-integrable function spaces $L^2(\mathcal{X})$ and $L^2(\mathcal{Y})$, we can build a minimizer of

$$
\min_{F \in \mathbb{R}^{m \times r}} \|K - FG^T\|_2 \quad \text{or} \quad \min_{f \in L^2(\mathcal{X})^r, g \in L^2(\mathcal{Y})^r} \|K(x, y) - f(x)^T g(y)\|_2
$$

by retaining only the $r$ largest singular values in the SVD of $K$ or $K(x, y)$.

In this paper, we present a new optimal low-rank approximation result with both conceptual and practical value. We summarize this result in the following theorem.

**Theorem 1.1.** The minimum of the maximum relative pointwise error in rank-$r$ approximations of the Cauchy kernel $1/(x - y)$,

$$
\epsilon_{r}(\mathcal{X}, \mathcal{Y}) := \min_{f \in \mathcal{F}(\mathcal{X})^r, g \in \mathcal{F}(\mathcal{Y})^r} \max_{x \in \mathcal{X}, y \in \mathcal{Y}} |1 - (x - y)f(x)^T g(y)|
$$

over sets $\mathcal{F}(\mathcal{X})$ and $\mathcal{F}(\mathcal{Y})$ of real-valued functions on compact real domains $\mathcal{X}$ and $\mathcal{Y}$ such that $\mathcal{X} > \mathcal{Y}$, exists and reduces to a minimization over real vectors $\tilde{x}$ and $\tilde{y}$,

$$
\epsilon_{r}(\mathcal{X}, \mathcal{Y}) = \min_{\tilde{x} \in \min(\mathcal{X}), \max(\mathcal{X})^r, \tilde{y} \in \min(\mathcal{Y}), \max(\mathcal{Y})^r} \max_{\tilde{x}_i < \tilde{x}_{i+1}, \tilde{y}_i < \tilde{y}_{i+1}} \left| \frac{h(x)}{h(y)} \right| \quad \text{for} \quad h(z) := \prod_{i=1}^r \frac{z - \tilde{x}_i}{z - \tilde{y}_i}.
$$

Minimizers of (1.1) and (1.2) are related by a skeleton decomposition defined as

$$
f(x)^T g(y) = C(x, \tilde{y})C(\tilde{x}, y)^{-1}C(\tilde{x}, \tilde{y}) \quad \text{for} \quad [C(x, y)]_{ij} := \frac{1}{x_i - y_j}.
$$

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Theorem 1.1 is an example of an integral kernel and error metric for which a skeleton decomposition [6] is optimal rather than the SVD. Extensions of this result to other kernels or error metrics are unlikely because of the specificity of its proof. However, skeleton decompositions may be superior to an SVD in similar circumstances.

The paper proceeds as follows. In section 2, we prove Theorem 1.1. In section 3, we briefly review the known analytical solution to (1.2) when \( \mathcal{X} \) and \( \mathcal{Y} \) are intervals. In section 4, we define and analyze a numerically stable form for (1.3). In section 5, we consider a numerical example for which the ratio of the error in a truncated SVD to the minimum error \( \epsilon_x(\mathcal{X}, \mathcal{Y}) \) diverges as \( \min(\mathcal{X}) \) approaches \( \max(\mathcal{Y}) \). In section 6, we conclude by suggesting several extensions and applications of Theorem 1.1.

2. Main proof. We decompose the proof into upper and lower bound lemmas and consolidate them with an existence proof for minimizers of (1.1) and (1.2). Until we prove existence, we consider infima rather than minima in (1.1) and (1.2).

Lemma 2.1. The minimax optimization in (1.2) is an upper bound of \( \epsilon_x(\mathcal{X}, \mathcal{Y}) \).

Proof. An analytical formula for the Cauchy matrix inverse [17],

\[
[C(x, y)^{-1}]_{ij} = \frac{\text{Res}(h, y_j) \text{Res}(1/h, x_j)}{y_i - y_j} \quad \text{for} \quad \text{Res}(f, x) = \lim_{y \to x} (y - x)f(y),
\]

indirectly relates (1.3) to \( h(z) \) by the complex residues of its simple roots and poles. By repeatedly using a partial fraction expansion to split products of poles into sums,

\[
\frac{1}{(x - z)(z - y)} = \frac{1}{x - y} \left[ \frac{1}{x - z} - \frac{1}{y - z} \right],
\]

and regrouping \( h(z) \) and \( 1/h(z) \) from their residue-pole representations,

\[
h(z) = 1 + \sum_{i=1}^{r} \frac{\text{Res}(h, y_i)}{z - y_i} \quad \text{and} \quad \frac{1}{h(z)} = 1 + \sum_{i=1}^{r} \frac{\text{Res}(1/h, x_i)}{z - x_i},
\]

we can simplify the rank-\( r \) approximation in (1.3) and directly relate it to \( h(z) \),

\[
f(x)^Tg(y) = \sum_{i=1}^{r} \sum_{j=1}^{r} \frac{\text{Res}(h, y_i)}{x - y_i} \frac{1}{y_i - x_j} \frac{\text{Res}(1/h, x_j)}{x_j - y} = \sum_{j=1}^{r} \frac{h(x) - h(x_j)}{x - x_j} \frac{\text{Res}(1/h, x_j)}{x_j - y} = h(x) \sum_{j=1}^{r} \frac{1}{x - x_j} \frac{\text{Res}(1/h, x_j)}{x_j - y} = \frac{h(x)}{x - y} \sum_{j=1}^{r} \left[ \frac{\text{Res}(1/h, x_j)}{x - x_j} - \frac{\text{Res}(1/h, x_j)}{y - x_j} \right] = \frac{1}{x - y} \left[ 1 - \frac{h(x)}{h(y)} \right].
\]

We restrict the minimization domain in (1.1) to (1.3) with ordered \( \tilde{x} \) and \( \tilde{y} \) domains, which is an upper bound that our simplified form of \( f(x)^Tg(y) \) reduces to

\[
\epsilon_x(\mathcal{X}, \mathcal{Y}) \leq \inf_{\tilde{x} \in [\min(\mathcal{X}), \max(\mathcal{X})]} \max_{\tilde{y} \in [\min(\mathcal{Y}), \max(\mathcal{Y})]} \left| \frac{h(x)}{h(y)} \right|.
\]

\( \square \)
Lemma 2.2. The minimax optimization in (1.2) is a lower bound of $\epsilon_r(\mathcal{X}, \mathcal{Y})$.

Proof. For $\min \{|\mathcal{X}|, |\mathcal{Y}|\} \leq r$, the trivial lower bound $\epsilon_r(\mathcal{X}, \mathcal{Y}) \geq 0$ is attained by any minimizer for which the elements of $\mathbf{x}$ cover $\mathcal{X}$ or the elements of $\mathbf{y}$ cover $\mathcal{Y}$.

Otherwise, we introduce auxiliary vectors $\mathbf{\alpha}$, $\mathbf{\theta}$, and $\mathbf{x}$ in (1.1) to expand it into

$$
\epsilon_r(\mathcal{X}, \mathcal{Y}) = \inf_{\alpha, \theta} \inf_{f \in \mathcal{F}(\mathcal{Y})^r} \sup_{x \in \mathcal{X}^{r+1}} \max_{i \in [r+1]} |\theta_i||1 - (x_i - y)|\mathbf{f}(y),
$$

where $x$ is replaced by $r + 1$ copies $x_i$, $\mathbf{f}_i$ is $\mathbf{F}$ with row $i$ removed for $[\mathbf{F}]_{i,j} := f_j(x_i)$, $\alpha_i \text{sgn}(\theta_i)$ is a constraint on det$(\mathbf{f}_i)$ that preserves the original minimization domain because it can take any real value, $|\theta_i|$ is a trivial weight of the generic form

$$
\max_{i \in [n]} |A_i| = \min_{w \in \mathbb{R}^n} \max_{i \in [n]} w_i |A_i|,
$$

and $[n]$ is the set of integers from 1 to $n$. We then use the max-min inequality,

$$
\inf_{b \in \mathcal{B}} \sup_{c \in \mathcal{C}} A(b, c) \geq \sup_{c \in \mathcal{C}} \inf_{b \in \mathcal{B}} A(b, c),
$$

to separate (2.4) into distinct inner and outer minimax optimizations,

$$
\epsilon_r(\mathcal{X}, \mathcal{Y}) \geq \inf_{\alpha, \theta} \sup_{f \in \mathcal{F}(\mathcal{X})^r} \inf_{x \in \mathcal{X}^{r+1}} \max_{i \in [r+1]} |\theta_i||1 - (x_i - y)|\mathbf{g}(y),
$$

where $\mathbf{f} \in \mathcal{F}(\mathcal{X})^r$ and $\mathbf{g} \in \mathcal{F}(\mathcal{Y})^r$ are replaced by $\mathbf{F} \in \mathbb{R}^{(r+1) \times r}$ and $\mathbf{g} \in \mathbb{R}^r$ to remove superfluous variables from the optimization. Since infima are invariant to removal of limit points from their domain, we restrict the domain to $\alpha_1 > 0$ for simplicity.

For fixed $\mathbf{F}$, the inner minimax problem in (2.6) is a linear program of the form

minimize $A$ subject to $-A \leq \theta_i(1 - (x_i - y)|\mathbf{f}(y)|) \leq A$ for $i \in [r+1]$.

As a linear program with $r$ variables and $r + 1$ pairs of constraints, it has minimizers that saturate one inequality per pair and reduce to a linear system that we can solve for $A$ using Cramer’s rule and cofactor expansions,

$$
A = \min_{s \in \{-1, 1\}} \left| \sum_{i=1}^{r+1} \frac{-\det(\mathbf{f}_i)}{x_i - y} \right| = \frac{\sum_{i=1}^{r+1} \alpha_i \theta_i}{\sum_{i=1}^{r+1} \alpha_i / x_i - y},
$$

where $s_i$ determines which constraint is saturated in each pair. By design, $\mathbf{\alpha}$ and $\mathbf{\theta}$ now encapsulate $\mathbf{F}$ and it can be removed from the remaining optimization problem,

$$
\epsilon_r(\mathcal{X}, \mathcal{Y}) \geq \inf_{\alpha, \theta} \sup_{f \in \mathcal{F}(\mathcal{X})^r} \inf_{x \in \mathcal{X}^{r+1}} \max_{i \in [r+1]} |\theta_i||1 - (x_i - y)|\mathbf{g}(y),
$$

which solves the inner minimax optimization in (2.6) unless $\alpha_i = 0$ for all $i$.

Applying a similar process as in the relaxation from (1.1) to (2.6), we introduce auxiliary vectors $\mathbf{\beta}$ and $\mathbf{y}$ into (2.7) and then relax it into inner and outer minimax
optimizations using the max-min inequality in (2.5). We replace \( y \) with \( r + 1 \) copies \( y_i \) and use \( \beta_i \) as trivial weights following a more complicated generic form

\[
\max_{i \in [n]} |A_i B_i| = \min_{w \in \mathbb{R}^n, i,j \in [n]} \max_{w_i > 0} \frac{u_{ij}}{w_i} |A_i B_j|.
\]

The subsequent transformation and relaxation of (2.7) into (2.8) and rewrite it using \( \tilde{A} \) Lagrange polynomial. Next, we maximize \( |x| \) and rewrite it using \( \tilde{x} \) variables and ignore the rest of them to relax the problem into

\[
\epsilon_r(\mathcal{X}, \mathcal{Y}) \geq \inf_{\alpha, \beta \in \mathbb{R}^{r+1}} \inf_{\theta \in \mathbb{R}^{r+1}} \sup_{j \in [r+1]} \max_{\beta_j \left| \sum_{l=1}^{r+1} \frac{\alpha_l \beta_l}{\beta_l x_l - y_l} \right|} \beta_j \left| \sum_{l=1}^{r+1} \frac{\alpha_l}{\beta_l x_l - y_l} \right|
\]

again isolates a linear program as its inner minimax optimization.

To solve the inner linear program in (2.8), we first relax it from \( r + 1 \) variables and \( 2r + 2 \) constraint pairs to \( r \) variables and \( r + 1 \) constraint pairs. Rescaling from \( \theta \) to \( \lambda \theta \) for \( \lambda \in (0, 1) \) can reduce the optimand until saturating a \( |\theta_i| \geq 1 \) constraint. We saturate \( |\theta_i| \geq 1 \) for some \( i \) and ignore the rest of them to relax the problem into

\[
\min A_i \quad \text{subject to} \quad -A_i \leq \frac{\alpha_i / \beta_j}{x_i - y_j} + \sum_{k \neq i}^{r+1} \frac{\alpha_k \beta_k / \beta_j}{x_k - y_j} \leq A_i \quad \text{for } j \in [r+1].
\]

We again solve the linear program using Cramer’s rule, cofactor expansions, and sign optimization and now simplify it with the Cauchy matrix determinant formula [17],

\[
A_i = \frac{\alpha_i \det(C(x, y))}{\sum_{j=1}^{r+1} \beta_j \det(C(x, y_j))} = \frac{\alpha_i \prod_{j \neq i}^{r+1} |x_i - x_j|}{\sum_{j=1}^{r+1} \beta_j \prod_{k=1}^{r+1} (x_k - y_j) |L_j(x, y)|},
\]

where \( x_i \) denotes a vector \( x \) with element \( i \) removed and \( L_i(x, y) := \prod_{j \neq i}^{r+1} \frac{x - x_j}{y - y_j} \) is a Lagrange polynomial. Next, we maximize \( A_i \) over \( i \) to obtain the tightest relaxation of (2.8) and rewrite it using \( \tilde{\alpha}_i := \alpha_i \prod_{j \neq i}^{r+1} |x_i - x_j| \) and \( \tilde{\beta}_i := \beta_i \prod_{j=i}^{r+1} (x_j - y_i) \) as

\[
\epsilon_r(\mathcal{X}, \mathcal{Y}) \geq \inf_{\tilde{\alpha}, \tilde{\beta} \in \mathbb{R}^{r+1}} \sup_{i,j \in [r+1]} \tilde{\alpha}_i \tilde{\beta}_j \cdot \frac{|\tilde{h}(x_i)|}{|\tilde{h}(y_j)|}
\]

for \( \tilde{h}(z) := \sum_{i=1}^{r+1} (-1)^i \tilde{\alpha}_i L_i(z, x) / \sum_{i=1}^{r+1} (-1)^i \tilde{\beta}_i L_i(z, y) \),

where \( \tilde{h}(z) \) is a rational function with simple roots and poles interleaved by \( x \) and \( y \) represented as a ratio of Lagrange polynomials with coefficients of alternating sign. Equivalently, we switch representations of the rational function to \( h(z) \) in (1.2) and revert the superfluous \( x \in \mathcal{X}^{r+1} \) and \( y \in \mathcal{Y}^{r+1} \) variables back to \( x \in \mathcal{X} \) and \( y \in \mathcal{Y} \),

\[
\epsilon_r(\mathcal{X}, \mathcal{Y}) \geq \inf_{\tilde{x} \in \text{min}(\mathcal{X}), \text{max}(\mathcal{X})} \max_{\tilde{y} \in \text{min}(\mathcal{Y}), \text{max}(\mathcal{Y})} \frac{|h(x)|}{|h(y)|}.
\]

\[ \square \]
Proof of Theorem 1.1. Lemma 2.1 and Lemma 2.2 prove the equality in (1.2), the proof of Lemma 2.1 establishes the relationship in (1.3) between minimizers of (1.1) and (1.2), and the proof of Lemma 2.2 establishes the existence of trivial minimizers for \( \min\{|X|,|Y|\} \leq r \). To complete this proof, we need to establish the existence of a minimizer for \( \min\{|X|,|Y|\} > r \). There must be a minimizer in the closure of the minimization domain of (1.2) that satisfies \( \tilde{x}_i \leq \hat{x}_{i+1} \) and \( \tilde{y}_i \geq \hat{y}_{i+1} \) for all \( i \), and we need to prove that \( \tilde{x}_i \neq \hat{x}_{i+1} \) and \( \tilde{y}_i \neq \hat{y}_{i+1} \). There is a correspondence [11] between minimizers \( h(z) \) of (1.2) and best Chebyshev rational approximants \( \tilde{s}(z) \) of \( s(z) \) such that \( s(x) = -1 \) for \( x \in \mathcal{X} \) and \( s(y) = 1 \) for \( y \in \mathcal{Y} \) whereby each local extrema of the residual error \( s(z) - \tilde{s}(z) \) corresponds to a local extrema from either \( h(x) \) for \( x \in \mathcal{X} \) or \( 1/h(y) \) for \( y \in \mathcal{Y} \). In turn, best Chebyshev rational approximants of a continuous real-valued function \( s(z) \) on a real interval \([\min(\mathcal{Y}), \max(\mathcal{X})]\) are well understood [15], and positive weight functions can arbitrarily suppress residual errors outside \( \mathcal{X} \cup \mathcal{Y} \). A best approximant \( \tilde{s}(z) \) exists, is unique, and is characterized by equioscillations of residual error between \( 2r+2 \) local extrema in \( \mathcal{X} \cup \mathcal{Y} \). These equioscillations bracket \( 2r \) roots in either \( h(x) \) for \( x \in [\min(\mathcal{X}), \max(\mathcal{X})] \) or \( 1/h(y) \) for \( y \in [\min(\mathcal{Y}), \max(\mathcal{Y})] \). These roots must be simple for an \( h(z) \) of degree \( r \), thus \( \tilde{x}_i \neq \hat{x}_{i+1} \) and \( \tilde{y}_i \neq \hat{y}_{i+1} \). 

We have not proved anything about uniqueness of minimizers to (1.1) and (1.2) because they are only unique in a very weak sense. For \( \min\{|X|,|Y|\} \leq r \), there is a unique minimizer of (1.2) only if \( |X| = |Y| = r \), but any minimizer of (1.1) forms a unique inner product, \( f(x)^T g(y) = C(x,y) \). For \( \min\{|X|,|Y|\} > r \), there is a unique minimizer of (1.2) from its correspondence to best Chebyshev rational approximants and thus a unique \( f(x)^T g(y) \) of the form in (1.3) that minimizes (1.1). However, this minimizer only attains its maximum error when \( x \) and \( y \) are restricted to a subset of \( r+1 \) points from \( \mathcal{X} \) and \( \mathcal{Y} \) that are local extrema of \( h(x) \) for \( x \in \mathcal{X} \) and \( 1/h(y) \) for \( y \in \mathcal{Y} \). We can perturb \( f(x)^T g(y) \) for \( x \) or \( y \) outside of this subset of points without changing the maximum error, therefore the minimizers of (1.1) do not form a unique \( f(x)^T g(y) \) unless they are constrained by (1.3) or the maximum error is zero.

3. Analytical solutions. Zolotarev’s third problem [20, 21] is a special case of (1.2) that has an analytical solution based on Jacobi elliptic functions,

\[
\epsilon_r([k',1],[-1,-k']) = \prod_{i=1}^{r} \left( \frac{1 - \sin(K(k)\frac{2i-1}{2r},k)}{1 + \sin(K(k)\frac{2i-1}{2r},k)} \right)^2 \leq 4 \exp\left(-2\pi \frac{K(k')}{K(k)} \right) \leq 4 \exp\left(-\frac{\pi^2}{\ln(4/k')} \right)
\]

for a modulus \( k \), complementary modulus \( k' = \sqrt{1-k^2} \), quarter period \( K \), and delta amplitude \( dn \). The first bound is tight for large \( r \), and the second bound is tight for small \( k' \) [1]. The corresponding residual roots and local extrema of (1.2) are

\[
\tilde{x}_i = -\hat{y}_i = \text{dn}(K(k)\frac{-i+1/2}{r},k) \quad \text{and} \quad \hat{x}_i = -\tilde{y}_i = \text{dn}(K(k)\frac{-i+1}{r},k).
\]

We can transform this solution to any disjoint pair of real intervals, \( \mathcal{X} = [x_{\min},x_{\max}] \) and \( \mathcal{Y} = [y_{\min},y_{\max}] \), by mapping roots and extrema with a Möbius transformation,

\[
M(z) = \frac{(1-k')(z+i)(z+x_{\min}+2k'(z-1)(y_{\max}-y_{\min}))}{(1-k')(z+i)(z+x_{\min})(1+k')(z-x_{\max})(y_{\min}-y_{\max}) + 2k'(z-1)(y_{\max}-y_{\min})},
\]

\[
k' = \frac{(\sqrt{(x_{\max}-x_{\min})(y_{\max}-y_{\min}) - (x_{\max}-x_{\min})(y_{\max}-y_{\min})^2})^2}{(x_{\min}-y_{\max})(x_{\max}-y_{\min})}.
\]
The value of $\epsilon_r$ is preserved by this domain transformation. This map also works for any $\mathcal{Y} = (-\infty, y_{\text{max}}] \cup [y_{\text{min}}, \infty)$ that is disjoint from $\mathcal{X}$ and can extend Theorem 1.1 to $\mathcal{Y} = \mathcal{Y}_+ \cup \mathcal{Y}_-$ that is closed but not compact and separated as $\mathcal{Y}_+ > \mathcal{X} > \mathcal{Y}_-$. Modern extensions of Zolotarev’s work include the study of Zolotarev numbers, which extends the minimax optimization in (1.2) to disjoint closed subsets $\mathcal{X}$ and $\mathcal{Y}$ of the complex plane and complex rational functions $h(z)$ with no constraints on the locations of their roots and poles. While no other analytical solutions are known for any real cases, there is a solution when $\mathcal{X}$ and $\mathcal{Y}$ are a pair of complex disks [18].

4. Stable form. The simple form of (1.3) is convenient for theoretical analysis, but it is numerically unstable in practical computations. For example, it is an exact decomposition of a Cauchy matrix for $|\mathcal{X}| = |\mathcal{Y}| = r$ into a product of the Cauchy matrix with its inverse and itself again. Although we can compute all the elements of a Cauchy matrix inverse to high relative accuracy, the matrix products are subject to a substantial accumulation of errors when the matrices have reduced numerical rank as a result of intermediate cancellations within small-valued inner products between large-norm vectors. To facilitate its practical use in computations, we can rearrange (1.3) into a numerically stable form that avoids explicit matrix inverses.

As an alternative to (1.3), we rearrange the kernel decomposition into

$$f(x)^T g(y) = p(x)^T C(\tilde{x}, \tilde{y}) q(y)$$

with implicit Cauchy matrix inverses encapsulated by interpolation vectors,

$$p(x) := C(\tilde{y}, \tilde{x})^{-1} C(\tilde{y}, x) \quad \text{and} \quad q(y) := C(\tilde{x}, \tilde{y})^{-1} C(\tilde{x}, y).$$

We can simplify $p(x)$ and $q(y)$ using (2.1), (2.2), and (2.3) into one of three forms,

$$p_i(x) = \frac{v(\tilde{x}_i)}{v(x)} L_i(x, \tilde{x}) = h(x) \frac{\text{Res}(1/h, \tilde{x}_i)}{x - \tilde{x}_i} = \frac{\text{Res}(1/h, \tilde{x}_i)}{x - \tilde{x}_i} \frac{\text{Res}(1/h, \tilde{x}_i)}{x - \tilde{x}_i} = 1 + \sum_{j=1}^{r} \frac{\text{Res}(1/h, \tilde{x}_i)}{x - \tilde{x}_i},$$

$$q_i(y) = \frac{w(\tilde{y}_i)}{w(y)} L_i(y, \tilde{y}) = \frac{1}{h(y)} \frac{\text{Res}(h, \tilde{y}_i)}{y - \tilde{y}_i} = \frac{\text{Res}(h, \tilde{y}_i)}{y - \tilde{y}_i} \frac{\text{Res}(h, \tilde{y}_i)}{y - \tilde{y}_i},$$

where $v(x)$ and $w(y)$ are degree-$r$ polynomials such that $h(z) = w(z) / v(z)$. The first form is a weighted Lagrange polynomial, the second form is an efficient modification, and the third form is its barycentric representation [2]. Thus (4.1) is an interpolation of the Cauchy kernel from a Cauchy matrix using rational basis functions, similar to interpolative matrix decompositions [5]. After precomputing their complex residues, the second form of $p(x)$ and $q(y)$ in (4.2) can be computed with $O(r)$ operations for each $x$ and $y$. The overall computation of each $p_i(x)$ and $q_i(y)$ is a multiplication or division of $4r$ binomials, which is backwards stable for floating-point arithmetic [9] assuming that the overflow or underflow of intermediate values and division by zero when $x = \tilde{x}_i$ or $y = \tilde{y}_i$ are carefully avoided.

If the elements of $\mathbf{p}(x)$ and $\mathbf{q}(y)$ both formed a partition of unity for each $x$ and $y$, then (4.1) could be computed to high relative accuracy because each term in the summation would be non-negative. This is not the case, and a condition number,

$$\kappa_r(\mathcal{X}, \mathcal{Y}) := \max_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} \frac{|\text{Res}(\mathbf{p}(x) \mathbf{q}(y))|}{|\text{Res}(\mathbf{p}(x) \mathbf{q}(y))|},$$
for \( \mathbf{x} \) and \( \mathbf{y} \) that minimize (1.2), quantifies the degree to which numerical accuracy is degraded by cancellations between \( p_i(x) \) and \( q_j(y) \) values of opposite sign, assuming that they are evaluated using the second form in (4.2) [9]. We can readily simplify the denominator because it is a bounded-error approximation of the Cauchy kernel,

\[
\kappa_r(\mathcal{X}, \mathcal{Y}) \leq \frac{1}{1 - \varepsilon_r(\mathcal{X}, \mathcal{Y})} \max_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} \frac{x - y}{x_i - y_j} \left| p_i(x)q_j(y) \right|.
\]

Similar to the proof of Lemma 2.1, we can use (2.2) to rearrange the summand into

\[
\frac{x - y}{x_i - y_j} p_i(x)q_j(y) = \left| \left( \frac{p_i(x) - h(x)}{y_j - x_i} \right) \left( q_j(y) - \frac{1}{h(y)} \frac{\text{Res}(h, \tilde{y}_j)}{x - y_j} \right) \right|,
\]

which has fewer opportunities to regroup terms. We then use the triangle inequality to split this summand into four terms, and simplify three of the terms using Hölder’s inequality and maximization-based relaxations to decouple variables,

\[
\sum_{j=1}^{r} \left| h(x) \frac{\text{Res}(1/h, \tilde{x}_i)}{y_j - x_i} q_j(y) \right| \leq \max_{y' \in \mathcal{Y}} \sum_{j=1}^{r} \left| h(x) \frac{\text{Res}(1/h, \tilde{x}_i)}{y' - x_i} q_j(y) \right|,
\]

\[
\sum_{j=1}^{r} \left| p_i(x) \frac{1}{h(y)} \frac{\text{Res}(h, \tilde{y}_j)}{x - y_j} \right| \leq \max_{x' \in \mathcal{X}} \sum_{j=1}^{r} \left| p_i(x') \frac{1}{h(y)} \frac{\text{Res}(h, \tilde{y}_j)}{x' - y_j} \right|,
\]

\[
\sum_{j=1}^{r} \left| \frac{h(x)}{h(y)} \frac{\text{Res}(1/h, \tilde{x}_i) \text{Res}(h, \tilde{y}_j)}{y_j - x_i} \right| \leq \max_{x' \in \mathcal{X}} \sum_{j=1}^{r} \left| \frac{h(x)}{h(y')} \frac{\text{Res}(1/h, \tilde{x}_i) \text{Res}(h, \tilde{y}_j)}{y' - x_i} \right|.
\]

Now the condition number bound can be regrouped and simplified into

\[
(4.4) \quad \kappa_r(\mathcal{X}, \mathcal{Y}) \leq \frac{[\Lambda(1/h, \mathcal{X}) + \Omega(1/h, \mathcal{Y})] + \varepsilon_r(\mathcal{X}, \mathcal{Y})[\Lambda(h, \mathcal{Y}) + \Omega(h, \mathcal{X})\varepsilon_r(\mathcal{X}, \mathcal{Y})]}{1 - \varepsilon_r(\mathcal{X}, \mathcal{Y})}
\]

with an even simpler approximation, \( \kappa_r(\mathcal{X}, \mathcal{Y}) \approx \Lambda(1/h, \mathcal{X})\Lambda(h, \mathcal{Y}) \) for \( \varepsilon_r(\mathcal{X}, \mathcal{Y}) \approx 0 \).

The Lebesgue constant of the weighted Lagrange polynomials in (4.2),

\[
(4.5) \quad \Lambda(1/h, \mathcal{X}) := \max_{x \in \mathcal{X}} \sum_{j=1}^{r} \left| \frac{\text{Res}(1/h, \tilde{x}_i)}{x - x_i} \right|,
\]

quantifies numerical stability of the interpolation basis. Superficially similar, \( \Omega(h, \mathcal{X}) \) quantifies the dependence of \( \max_{x \in \mathcal{X}} |h(x)| \) on the signs of its complex residues,

\[
(4.6) \quad \Omega(h, \mathcal{X}) := \max_{x \in \mathcal{X}} \sum_{j=1}^{r} \left| \frac{\text{Res}(h, \tilde{y}_j)}{x - y_j} \right|.
\]

The numerical stability of (4.1) depends upon the slow growth of \( \Lambda(1/h, \mathcal{X}), \Lambda(h, \mathcal{Y}), \Omega(h, \mathcal{X})\varepsilon_r(\mathcal{X}, \mathcal{Y}), \) and \( \Omega(1/h, \mathcal{Y})\varepsilon_r(\mathcal{X}, \mathcal{Y}) \) with increasing \( r \).

Lebesgue constants of rational interpolants are an active area of research [3, 10], but all available theoretical results make assumptions about interpolation points and weights that do not immediately apply here. We empirically gauge our expectations by calculating \( \Lambda(1/h, \mathcal{X}) \) and \( \Omega(h, \mathcal{X}) \) for \( h(z) \) constructed from analytical solutions.
in section 3. In this example, $\Lambda(h, \mathcal{Y}) = \Lambda(1/h, \mathcal{X})$ and $\Omega(1/h, \mathcal{Y}) = \Omega(h, \mathcal{X})$ because of symmetry. In the $k' \to 1$ limit, the roots and poles of $h(z)$ become the Chebyshev nodes of the first kind scaled and shifted from $[-1, 1]$ to $[k', 1]$ and $[-1, -k']$, and the Lagrange function weights in (4.2) become constant over the approximation domain. Lebesgue constants of Lagrange polynomials at Chebyshev nodes are well understood [4], and for large $r$ they are known to have the asymptotic form

\[
\lim_{k' \to 1} \Lambda(1/h, [k', 1]) \sim \frac{2}{\pi} \log r + \frac{2}{\pi} \left( \gamma + \log \frac{8}{\pi} \right)
\]

where $\gamma$ is Euler’s constant. The maximum in (4.5) is known to occur at both $k'$ and 1 in this limit, and we observe the maximum at $k'$ to persist in general. We visualize the dependence of $\Lambda(1/h, \mathcal{X})$ on $r$ and $k'$ in Figure 4.1, which has the same apparent large-$r$ asymptotic as (4.7) with a logarithmic growth of the constant offset in $1/k'$,

\[
\Lambda(1/h, [k', 1]) \sim \frac{2}{\pi} \log r + \frac{2}{\pi} \left( \gamma + \log \frac{8}{\pi} \right) + \lambda \left( \log \frac{1}{k'} \right).
\]

We observe similar but somewhat simpler behavior in $\Omega(h, \mathcal{X})$. Its value diverges for large $r$, but its product with $\epsilon_r(\mathcal{X}, \mathcal{Y})$ is asymptotically independent of $r$,

\[
\Omega(h, [k', 1]) \epsilon_r([k', 1], [-1, -k']) \sim \omega \left( \log \frac{1}{k'} \right).
\]

We can accurately fit the data on $\lambda(x)$ and $\omega(x)$ with simple rational approximants,

\[
\lambda(x) \approx 0.312x \frac{4.4 + x}{11 + x} \quad \text{and} \quad \omega(x) \approx 0.319x \frac{0.1 + x}{0.9 + x}.
\]

Thus we can readily describe some of the behavior of $\Lambda(1/h, \mathcal{X})$ and $\Omega(h, \mathcal{X})$ without undergoing the more challenging task of explaining it. This suffices to establish the numerical stability of (4.1) for practical applications of the solutions in section 3.

\[
\text{Fig. 4.1. Values of (4.5) and (4.6) for } \mathcal{X} = [k', 1], \mathcal{Y} = [-1, -k'], \text{ and } h(z) \text{ that minimizes (1.2).}
\]
Future use of Theorem 1.1 in practical computations may be based on numerical solutions to (1.2). After generating a numerical solution, it would be straightforward to calculate the bound on $\kappa_r(\mathcal{X}, \mathcal{Y})$ in (4.4). Although not absolutely essential, more theoretical results on error analysis could be a useful guide to practice. Proof of the asymptotic results in (4.8) and (4.9) may be achieved by extending known proofs for Chebyshev nodes [4] based on properties of trigonometric functions to the analogous Jacobi elliptic functions. An even more useful theoretical result would be a bound on $\kappa_r(\mathcal{X}, \mathcal{Y})$ that depends only on $\epsilon_r(\mathcal{X}, \mathcal{Y})$ and basic properties of $\mathcal{X}$ and $\mathcal{Y}$. Ideally, we would like the minimization of low-rank approximation errors to be synergistic with the minimization of arithmetic rounding errors, which is what would be expressed by such a bound. For example, a trivial bound on low-rank approximation errors,

\begin{equation}
\epsilon_r(\mathcal{X}', \mathcal{Y}') \leq \epsilon_r(\mathcal{X}, \mathcal{Y}) \quad \text{for} \quad \mathcal{X}' \subseteq \mathcal{X} \quad \text{and} \quad \mathcal{Y}' \subseteq \mathcal{Y},
\end{equation}

does not obviously have a corresponding bound on the condition number. We cannot immediately discount the possibility that a small reduction in $\epsilon_r(\mathcal{X}', \mathcal{Y}')$ relative to a solution in section 3 causes a substantial increase in $\kappa_r(\mathcal{X}', \mathcal{Y}')$ in some cases, which could negate the advantages of numerical solutions over analytical solutions.

5. Numerical example. The two possible benefits of (1.3) in practice are its analytical form and its optimality for (1.1). However, if a truncated SVD is close to optimal, then this second benefit might be irrelevant. The SVD is a flexible tool, and rank-$r$ approximations of $C(x, y)$ can be constructed using weights $W_L$ and $W_R$ as

\begin{equation}
W_L^{-1}W_L C(x, y) W_R W_R^{-1} = W_L^{-1} UDV^T W_R^{-1} \approx W_L^{-1} U_r D_r V_r^T W_R^{-1}
\end{equation}

where $U_r D_r V_r^T$ is the weighted SVD truncated to its $r$ largest singular values. Any rank-$r$ approximation can be constructed in this manner if $W_L$ and $W_R$ are chosen without constraints and with knowledge of the target. However, we are interested in the ability of a truncated SVD to circumvent solving (1.2) and constructing (1.3), so we will artificially limit our knowledge of the target in choosing $W_L$ and $W_R$.

As an example, we consider Cauchy matrices parameterized by $k' \in (0, 1)$ as

\begin{equation}
C(x, y) \in \mathbb{R}^{n \times n} \quad \text{for} \quad x_i = -y_i = (k')^{(n-i)/(n-1)} \quad \text{and} \quad n = 1000.
\end{equation}

For simplicity, we use the analytical solutions in section 3 to approximate minimizers of (1.2) for these matrices, which is accurate for $r \ll n$. Also, we simplify the choice of $W_L$ and $W_R$ by restricting them to be positive-definite diagonal matrices.

Our comparison of low-rank approximations is simplified by the fact that each is optimal with respect to a different matrix norm. The skeleton decomposition in (1.3) minimizes the maximum relative pointwise error in (1.1) and the truncated SVD in (5.1) minimizes a weighted 2-norm. These norms of a matrix $A$ bound one another,

\begin{equation}
\eta_1 \|W_L A W_R\|_2 \leq \max_{i,j} |(x_i - y_j) [A]_{ij}| \leq \frac{1}{\eta_2} \|W_L A W_R\|_2,
\end{equation}

with multiplicative constants that quantify the most extreme cases,

$$\eta_1 := \min_{B \in \mathbb{R}^{n \times n}} \frac{\max_{i,j} |(x_i - y_j) [B]_{ij}|}{\|W_L B W_R\|_2} \quad \text{and} \quad \eta_2 := \min_{B \in \mathbb{R}^{n \times n}} \frac{\|W_L B W_R\|_2}{\max_{i,j} |(x_i - y_j) [B]_{ij}|}.$$

Matrix norms are equivalent, which means that $\eta_1$ and $\eta_2$ must be nonzero. If $A$ in (5.3) is the residual matrix of a rank-$r$ approximation, $C(x, y) - FG^T$, then we can
minimize the upper and lower bounds with the truncated SVD in (5.1) to construct both an interval of values for the minimum of the maximum relative pointwise error and a rank-r approximation with an error in that interval. Short intervals, \( \eta_1 \eta_2 \approx 1 \), correspond to optimal low-rank approximations with respect to either norm having similar errors and thus good interoperability. If \( \eta_1 \eta_2 \ll 1 \), then it is possible to have substantial differences between these optimal low-rank approximations.

We choose \( W_L \) and \( W_R \) to maximize \( \eta_1 \eta_2 \) and thus the interoperability between (1.3) and (5.1). However, we must make several approximations for the optimal \( W_L \) and \( W_R \) to have closed-form solutions. We calculate \( \eta_1 \) and \( \eta_2 \) by changing variables to \( A := W_L BW_R \) with the constraint \( \|A\|_2 = 1 \) and further restricting \( A \) to a single nonzero matrix element, which is exact for \( \eta_2 \) but only an upper bound for \( \eta_1 \),

\[
\eta_1 \leq \min_{i,j} |(x_i - y_j)[W^{-1}_L]_{i,i}[W^{-1}_R]_{j,j}|
\]

\[
\eta_2^{-1} = \max_{i,j} |(x_i - y_j)[W^{-1}_L]_{i,i}[W^{-1}_R]_{j,j}|
\]

We maximize the corresponding upper bound on \( \eta_1 \eta_2 \) by minimizing the deviation of its optimands from one, which is equivalent to (1.1) for \( r = 1 \). The final simplifying approximation is to use the analytical solution from section 3, which results in

\[
(W_L)_{i,i} = x_i + \sqrt{k'} \quad \text{and} \quad (W_R)_{i,i} = y_i + \sqrt{k'}
\]

with \( \eta_1 \eta_2 \leq 2\sqrt{k'} \). This improves upon \( \eta_1 \eta_2 \leq k' \) for \( W_L = W_R = I \).

Accounting for the flexibility of the SVD, we compare the suboptimality of the unweighted 2-norm error of minimizers of (1.1) with the maximum relative pointwise error of a truncated SVD weighted by (5.4). As shown in Figure 5.1, these errors all have an asymptotic exponential decay in \( r \) with the same rate, which is an inevitable

![Fig. 5.1. Behavior of the maximum relative pointwise error and unweighted 2-norm error in rank-r approximations of (5.2) based on skeleton decompositions that minimize (1.1) and truncated SVDs. The maximum relative pointwise error of the unweighted SVD (gray dots and line) is reduced by a weighted SVD in (5.1) for weights in (5.4). The error floors (dotted lines) are a product of the floating-point rounding error, \( 2^{-52} \), and either \( ||C(x,y)||_2 \) for the SVD or \( \kappa_r([k',1],[-1,-k']) \) in (4.3) for the skeleton decomposition, plotted for \( r = 50 \). For each \( k' \), the error ratios are measured at the \( r \) value for which the 2-norm error in the SVD is just above 100x its error floor.](image-url)
result of norm equivalence. This decay rate set by \( \epsilon_r([k', 1], [-1, -k']) \) is consistent with upper bounds on the decay of singular values of Cauchy matrices \([1]\). Because the equivalence between norms in (5.3) is weak at small \( k' \) and we are limited in how much we can probe the asymptotic regime by error floors, we are not able to extract accurate estimates of asymptotic error ratios. For the accessible large-\( r \) error ratios, there is apparent algebraic decay in \( k' \) over ten orders of magnitude. The observed decay is \( \propto (k')^{-0.47} \) for the unweighted 2-norm, and it reduces to \( \propto (k')^{-0.15} \) for the weighted 2-norm. Thus the truncated SVD can be improved substantially with only limited access to optimal solutions and restricted weights, but it remains suboptimal for the maximum relative pointwise error with an error ratio that appears to diverge in the \( k' \to 0 \) limit. The skeleton decomposition retains a practical advantage.

6. Conclusions. The connection between (1.1) and (1.2) was recently suggested \([1]\) for its simplicity and utilization of results in rational approximation theory. Here we have proven (1.3) to be an optimal choice over real-valued functions rather than merely a convenient choice. It connects Zolotarev’s work \([20, 21]\) on optimal rational approximation of functions to optimal low-rank approximation of operators. Cauchy kernels are special because their skeleton decompositions \([6]\) coincide with rational interpolants. For applications in which the maximum relative pointwise error is the most relevant error metric, this simple result also has a quantitative advantage over an SVD. This paper is one instance of the general activity of refining and optimizing elementary approximation results for possible use in fast numerical algorithms.

There are several ways in which the results of this paper might be extended and expanded. Theorem 1.1 does not apply to complex-valued \( \mathcal{X}, \mathcal{Y}, \tilde{x}, \tilde{y} \), but (1.2) remains an upper bound on \( \epsilon_r(\mathcal{X}, \mathcal{Y}) \). The optimized roots and poles of \( h(z) \) are not necessarily simple in the complex case. Theorem 1.1 can be extended by including a positive separable weight function \( w_1(x)w_2(y) \) in the error metric. Most of the proof of Lemma 2.2 can be adapted to other kernel functions, but it is not clear that this can be leveraged into a useful result. As noted in section 4, (4.8) and (4.9) probably can be proven using known properties of Jacobi elliptic functions and existing proofs of Lebesgue constant asymptotics for Chebyshev nodes \([4]\). Finally, practical use of Theorem 1.1 would benefit from efficient and reliable access to numerical solutions of (1.2), (4.5), and (4.6) for more general \( \mathcal{X} \) and \( \mathcal{Y} \) such as finite sets of intervals.

The results of this paper have three imminent applications. First, there are fast algorithms for electronic structure simulation \([14]\) that need rational approximations on a real interval of multiple functions with poles on the imaginary axis. Analytical solutions in section 3 can be applied here by using a degree-doubling transformation \( z' = \sqrt{z} \) to map the approximation domains from \( \mathcal{X} = [0, 1] \) and \( \mathcal{Y} = (-\infty, -k] \) into \( \mathcal{X}' = [-1, 1] \) and \( \mathcal{Y}' = \{iy : y \in (-\infty, -\sqrt{k}] \cup [\sqrt{k}, \infty)\} \). This avoids function-specific numerical optimization \([16]\) and can be consolidated with low-rank approximations of energy denominators \([19]\). Second, hierarchical factorization of real Cauchy matrices with high relative accuracy is possible by recursively partitioning a matrix as

\[
\mathbf{C}(\mathbf{x}, \mathbf{y}) = \begin{bmatrix}
\mathbf{C}(\mathbf{x}_1, \mathbf{y}_1) & \mathbf{C}(\mathbf{x}_1, \mathbf{y}_2) \\
\mathbf{C}(\mathbf{x}_2, \mathbf{y}_1) & \mathbf{C}(\mathbf{x}_2, \mathbf{y}_2)
\end{bmatrix}
\]

such that Theorem 1.1 can be applied to the off-diagonal matrix blocks as the process is recursed on the diagonal matrix blocks. Third, dimensional reduction algorithms for sparse symmetric eigenvalue problems \([12]\) use the Cauchy kernel in various ways for spectral filtering. Theorem 1.1 can improve on efficiency and accuracy of spectral filtering, enabling its use as a reliable primitive in new eigenvalue algorithms.
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