

ON THE SINGULAR VALUES OF MATRICES WITH DISPLACEMENT STRUCTURE

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Abstract. Matrices with displacement structure such as Pick, Vandermonde, and Hankel matrices appear in a diverse range of applications. In this paper, we use an extremal problem involving rational functions to derive explicit bounds on the singular values of such matrices. For example, we show that the k th singular value of a real $n \times n$ positive definite Hankel matrix, H_n , is bounded by $C\rho^{-k/\log n}\|H\|_2$ with explicitly given constants $C > 0$ and $\rho > 1$, where $\|H_n\|_2$ is the spectral norm. This means that a real $n \times n$ positive definite Hankel matrix can be approximated, up to an accuracy of $\epsilon\|H_n\|_2$ with $0 < \epsilon < 1$, by a rank $\mathcal{O}(\log n \log(1/\epsilon))$ matrix. Analogous results are obtained for Pick, Cauchy, real Vandermonde, Löwner, and certain Krylov matrices.

Key words. singular values, displacement structure, Zolotarev, rational

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1. Introduction. Matrices with rapidly decaying singular values frequently appear in computational mathematics. Such matrices are numerically of low rank and this is exploited in applications such as particle simulations [23], model reduction [2], boundary element methods [25], and matrix completion [17]. However, it can be theoretically challenging to fully explain why low rank techniques are so effective in practice. In this paper, we derive explicit bounds on the singular values of matrices with displacement structure and in doing so justify many of the low rank techniques that are being employed on such matrices.

Let $X \in \mathbb{C}^{m \times n}$ with $m \geq n$, $A \in \mathbb{C}^{m \times m}$, and $B \in \mathbb{C}^{n \times n}$, we say that X has an (A, B) -displacement rank of ν if X satisfies the Sylvester matrix equation given by

$$(1) \quad AX - XB = MN^*,$$

for some matrices $M \in \mathbb{C}^{m \times \nu}$ and $N \in \mathbb{C}^{n \times \nu}$. Matrices with displacement structure include Toeplitz ($\nu = 2$), Hankel ($\nu = 2$), Cauchy ($\nu = 1$), Krylov ($\nu = 1$), and Vandermonde ($\nu = 1$) matrices, as well as Pick ($\nu = 2$), Sylvester ($\nu = 2$), and Löwner ($\nu = 2$) matrices. Fast algorithms for computing matrix-vector products and for solving systems of linear equations can be derived for many of these matrices by exploiting (1.1) [26, 29].

In this paper, we use the displacement structure to derive explicit bounds on the singular values of matrices that satisfy (1.1) by using an extremal problem for rational functions from complex approximation theory. In particular, we prove that the following inequality holds (see Theorem 2.1):

$$(2) \quad \sigma_{j+\nu k}(X) \leq Z_k(E, F)\sigma_j(X), \quad 1 \leq j + \nu k \leq n,$$

where $\sigma_1(X), \dots, \sigma_n(X)$ denote the singular values of X and $Z_k(E, F)$ is the Zolotarev number (1.4) for complex sets E and F that depend on A and B . Researchers have previously exploited the connection between the Sylvester matrix equation and Zolotarev numbers for selecting algorithmic parameters in the Alternating Direction Implicit

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Matrix class	Notation	Singular value bound	Ref.
Pick	P_n	$\sigma_{1+2k}(P_n) \leq C_1 \rho_1^{-k} \ P_n\ _2$	Sec. 4.1
Cauchy	$C_{m,n}$	$\sigma_{1+k}(C_{m,n}) \leq C_2 \rho_2^{-k} \ C_{m,n}\ _2$	Sec. 4.2
Löwner	L_n	$\sigma_{1+2k}(L_n) \leq C_3 \rho_3^{-k} \ L_n\ _2$	Sec. 4.3
Krylov, Herm. arg.	$K_{m,n}$	$\sigma_{1+2k}(K_{m,n}) \leq C_4 \rho_4^{-k/\log n} \ K_{m,n}\ _2$	Sec. 5.1
Real Vandermonde	$V_{m,n}$	$\sigma_{1+2k}(V_{m,n}) \leq C_5 \rho_5^{-k/\log n} \ V_{m,n}\ _2$	Sec. 5.1
Pos. semidef. Hankel	H_n	$\sigma_{1+2k}(H_n) \leq C_6 \rho_6^{-k/\log n} \ H_n\ _2$	Sec. 5.2

TABLE 1

Summary of the bounds proved on the singular values of matrices with displacement structure. For the singular value bounds to be valid for $C_{m,n}$ and L_n mild “separation conditions” must hold (see Section 4). The numbers ρ_j and C_j for $j = 1, \dots, 6$ are given explicitly in their corresponding sections.

(ADI) method [8, 13, 27], and others have demonstrated that the singular values of matrices satisfying certain Sylvester matrix equations have rapidly decaying singular values [2, 4, 35]. Here, we derive explicit bounds on all the singular values of structured matrices. Table 1.1 summarizes our main singular value bounds.

Not every matrix with displacement structure is numerically of low rank. For example, the identity matrix is a full rank Toeplitz matrix and the exchange matrix¹ is a full rank Hankel matrix. The properties of A and B in (1.1) are crucial. If A and B are normal matrices, then one expects X to be numerically of low rank only if the eigenvalues of A and B are well-separated (see Theorem 2.1). If A and B are both not normal, then as a general rule spectral sets for A and B should be well-separated (see Corollary 2.2).

By the Eckart–Young Theorem [43, Theorem 2.4.8], singular values measure the distance in the spectral norm from X to the set of matrices of a given rank, i.e.,

$$\sigma_j(X) = \min \{ \|X - Y\|_2 : Y \in \mathbb{C}^{m \times n}, \text{rank}(Y) = j - 1 \}.$$

For an $0 < \epsilon < 1$, we say that the ϵ -rank of a matrix X is k if k is the smallest integer such that $\sigma_{k+1}(X) \leq \epsilon \|X\|_2$. That is,

$$(3) \quad \text{rank}_\epsilon(X) = \min_{k \geq 0} \{ k : \sigma_{k+1}(X) \leq \epsilon \|X\|_2 \}.$$

Thus, we may approximate X to a precision of $\epsilon \|X\|_2$ by a rank $k = \text{rank}_\epsilon(X)$ matrix.

An immediate consequence of explicit bounds on the singular values of certain matrices is a bound on the ϵ -rank. Table 1.2 summarizes our main upper bounds on the ϵ -rank of matrices with displacement structure.

Zolotarev numbers have already proved useful for deriving tight bounds on the condition number of matrices with displacement structure [5, 6]. For example, the first author proved that a real $n \times n$ positive definite Hankel matrix, H_n , with $n \geq 3$, is exponentially ill-conditioned [6]. That is,

$$\kappa_2(H_n) = \frac{\sigma_1(H_n)}{\sigma_n(H_n)} \geq \frac{\gamma^{n-1}}{16n}, \quad \gamma \approx 3.210,$$

¹The $n \times n$ exchange matrix X is obtained by reversing the order of the rows of the $n \times n$ identity matrix, i.e., $X_{n-j+1,j} = 1$ for $1 \leq j \leq n$.

Matrix class	Notation	Upper bound on $\text{rank}_\epsilon(X)$	Ref.
Pick	P_n	$2\lceil \log(4b/a) \log(4/\epsilon)/\pi^2 \rceil$	Sec. 4.1
Cauchy	$C_{m,n}$	$\lceil \log(16\gamma) \log(4/\epsilon)/\pi^2 \rceil$	Sec. 4.2
Löwner	L_n	$2\lceil \log(16\gamma) \log(4/\epsilon)/\pi^2 \rceil$	Sec. 4.3
Krylov, Herm. arg.	$K_{m,n}$	$2\lceil 4\log(8\lfloor n/2 \rfloor/\pi) \log(4/\epsilon)/\pi^2 \rceil + 2$	Sec. 5.1
Real Vandermonde	$V_{m,n}$	$2\lceil 4\log(8\lfloor n/2 \rfloor/\pi) \log(4/\epsilon)/\pi^2 \rceil + 2$	Sec. 5.1
Pos. semidef. Hankel	H_n	$2\lceil 2\log(8\lfloor n/2 \rfloor/\pi) \log(16/\epsilon)/\pi^2 \rceil + 2$	Sec. 5.2

TABLE 2

Summary of the upper bounds proved on the ϵ -rank of matrices with displacement structure. For the bounds above to be valid for $C_{m,n}$ and L_n mild “separation conditions” must hold (see Section 4). The number is the absolute value of the cross-ratio of a, b, c , and d , see (4.7). The first three rows show an ϵ -rank of at most $\mathcal{O}(\log \gamma \log(1/\epsilon))$ and the last three rows show an ϵ -rank of at most $\mathcal{O}(\log n \log(1/\epsilon))$.

and that this bound cannot be improved by more than a factor of n times a modest constant. The Hilbert matrix given by $(H_n)_{jk} = 1/(j+k-1)$, for $1 \leq j, k \leq n$, is the classic example of an exponentially ill-conditioned positive definite Hankel matrix [44, eqn. (3.35)]. Similar exponential ill-conditioning has been shown for certain Krylov matrices and real Vandermonde matrices [6].

This paper extends the application of Zolotarev numbers to deriving bounds on the singular values of matrices with displacement structure, not just the condition number. The bounds we derive are particularly tight for $\sigma_j(X)$, where j is small with respect to n . Improved bounds on $\sigma_j(X)$ when $j/n \rightarrow c \in (0, 1)$ may be possible with the ideas found in [9]. Nevertheless, our interest here is to justify the application of low rank techniques on matrices with displacement structure by proving that such matrices are often well-approximated by low rank matrices. The bounds that we derive are sufficient for this purpose.

For an integer k , let $\mathcal{R}_{k,k}$ denote the set of irreducible rational functions of the form $p(x)/q(x)$, where p and q are polynomials of degree at most k . Given two closed disjoint sets $E, F \subset \mathbb{C}$, the corresponding Zolotarev number, $Z_k(E, F)$, is defined by

$$(4) \quad Z_k(E, F) := \inf_{r \in \mathcal{R}_{k,k}} \frac{\sup_{z \in E} |r(z)|}{\inf_{z \in F} |r(z)|},$$

where the infimum is attained for some extremal rational function. As a general rule, the number $Z_k(E, F)$ decreases rapidly to zero with k if E and F are sets that are disjoint and well-separated. Zolotarev numbers satisfy several immediate properties: for any sets E and F and integers k, k_1 , and k_2 , one has $Z_0(E, F) = 1$, $Z_k(E, F) = Z_k(F, E)$, $Z_{k+1}(E, F) \leq Z_k(E, F)$ and $Z_{k_1+k_2}(E, F) \leq Z_{k_1}(E, F)Z_{k_2}(E, F)$. They also satisfy $Z_k(E_1, F_1) \leq Z_k(E_2, F_2)$ if $E_1 \subseteq E_2$ and $F_1 \subseteq F_2$ as well as $Z_k(E, F) = Z_k(T(E), T(F))$, where T is any Möbius transformation [1]. As $k \rightarrow \infty$ the value for $Z_k(E, F)$ is known asymptotically to be

$$\lim_{k \rightarrow \infty} (Z_k(E, F))^{1/k} = \exp \left(-\frac{1}{\text{cap}(E, F)} \right),$$

where $\text{cap}(E, F)$ is the logarithmic capacity of a condenser with plates E and F [21].

To readers that are not familiar with Zolotarev numbers, it may seem that (1.2) trades a difficult task of directly bounding the singular values of a matrix X with a more abstract task of understanding the behavior of $Z_k(E, F)$. However, Zolotarev numbers have been extensively studied in the literature [1, 21, 45] and for certain sets E and F the extremal rational function is known explicitly [1, Sec. 50] (see Section 3). Our major challenge for bounding singular values is to carefully select sets E and F so that one can use complex analysis and Möbius transformations to convert the associated extremal rational approximation problem in (1.4) into one that has an explicit bound.

The paper is structured as follows. In Section 2 we prove (1.2), giving us a bound on the singular values of matrices with displacement structure in terms of Zolotarev numbers. In Section 3 we derive new sharper bounds on $Z_k([-b, -a], [a, b])$ when $0 < a < b < \infty$ by correcting an infinite product formula from Lebedev (see Theorem 3.1 and Corollary 3.2). In Section 4 we derive explicit bounds on the singular values of Pick, Cauchy, and Löwner matrices. In Section 5 we tackle the challenging task of showing that all real Vandermonde and positive definite Hankel matrices have rapidly decaying singular values and can be approximated, up to an accuracy of $0 < \epsilon < 1$, by a rank $\mathcal{O}(\log n \log(1/\epsilon))$ matrix. In Appendix A we further detail the unfortunate consequences of the erroneous infinite product formula from Lebedev and present corrected results.

2. The singular values of matrices with displacement structure and Zolotarev numbers. Let X be an $m \times n$ matrix with $m \geq n$ that satisfies (1.1). We show that the singular values of X can be bounded from above in terms of Zolotarev numbers. First, we assume that A and B in (1.1) are normal matrices and later remove this assumption in Corollary 2.2. In Theorem 2.1 the spectrum (set of eigenvalues) of A and B is denoted by $\sigma(A)$ and $\sigma(B)$, respectively.²

THEOREM 1. *Let $A \in \mathbb{C}^{m \times m}$ and $B \in \mathbb{C}^{n \times n}$ be normal matrices with $m \geq n$ and let E and F be complex sets such that $\sigma(A) \subseteq E$ and $\sigma(B) \subseteq F$. Suppose that the matrix $X \in \mathbb{C}^{m \times n}$ satisfies*

$$AX - XB = MN^*, \quad M \in \mathbb{C}^{m \times \nu}, \quad N \in \mathbb{C}^{n \times \nu},$$

where $1 \leq \nu \leq n$ is an integer. Then, for $j \geq 1$ the singular values of X satisfy

$$\sigma_{j+\nu k}(X) \leq Z_k(E, F) \sigma_j(X), \quad 1 \leq j + \nu k \leq n,$$

where $Z_k(E, F)$ is the Zolotarev number in (1.4).

Proof. Let $p(z)$ and $q(z)$ be polynomials of degree at most k . First, we show that

$$(5) \quad \text{rank}(p(A)Xq(B) - q(A)Xp(B)) \leq \nu k, \quad \nu = \text{rank}(AX - XB).$$

²The statement of Theorem 2.1 was presented by the first author at the Cortona meeting on Structured Numerical Linear Algebra in 2008 [7] as well as several other locations. The statement has not appeared in a publication by the first (or second) author before. Similar statements based on the presentation have appeared in [36, Theorem 2.1.1], [37, Theorem 4], and most recently [12, Theorem 4.2].

128 Suppose that $p(z) = z^s$ and $q(z) = z^t$, where $k \geq s \geq t$, then

$$\begin{aligned}
 p(A)Xq(B) - q(A)Xp(B) &= A^t (A^{s-t}X - XB^{s-t}) B^t \\
 &= \sum_{j=0}^{s-t-1} A^{t+j}(AX - XB)B^{s-1-j} \\
 &= \sum_{j=0}^{s-t-1} (A^{t+j}M) (N^*B^{s-1-j}).
 \end{aligned}$$

130 In the last sum we have terms of the form $(A^\ell M)(N^*B^\wp)$, with $0 \leq \ell, \wp \leq k-1$. By
 131 adding together the terms occurring in $p(A)Xq(B) - q(A)Xp(B)$ for general degree k
 132 polynomials p and q , we conclude that there exist coefficients $c_{\ell, \wp} \in \mathbb{C}$ such that

$$p(A)Xq(B) - q(A)Xp(B) = \sum_{\ell, \wp=0}^{k-1} c_{\ell, \wp} (A^\ell M) (N^*B^\wp).$$

134 This shows that the rank of $p(A)Xq(B) - q(A)Xp(B)$ is bounded above by k times
 135 the number of columns of M , proving (2.1).

136 Now, let $r(z) = p(z)/q(z)$, where p and q are polynomials of degree k so that
 137 $r(z)$ is the extremal rational function for the Zolotarev number in (1.4). This means
 138 that $p(z)$ and $q(z)$ are not zero on F and E , respectively, so that $p(B)$ and $q(A)$ are
 139 invertible matrices. From (2.1) we know that $\Delta = p(A)Xq(B) - q(A)Xp(B)$ has rank
 140 at most νk and hence, the matrix

$$Y = -q(A)^{-1}\Delta p(B)^{-1} = X - r(A)Xr(B)^{-1}$$

142 is of rank at most νk . Let X_j be the best rank $j-1$ approximation to X in $\|\cdot\|_2$ and
 143 let $Y_{j-1} = r(A)X_{j-1}r(B)^{-1}$. Since Y_{j-1} is of rank at most $j-1$, $Y + Y_{j-1}$ is of rank
 144 at most $j + \nu k - 1$. This implies that

$$\begin{aligned}
 \sigma_{j+\nu k}(X) &\leq \|X - Y - Y_{j-1}\|_2 \\
 &= \|r(A)(X - X_{j-1})r(B)^{-1}\|_2 \\
 &\leq \|r(A)\|_2 \|r(B)^{-1}\|_2 \sigma_j(X),
 \end{aligned}$$

146 where in the last inequality we used the relation $\sigma_j(X) = \|X - X_{j-1}\|_2$. Finally,
 147 since A and B are normal we have $\|r(A)\|_2 \leq \sup_{z \in \sigma(A)} |r(z)|$ and $\|r(B)^{-1}\|_2 \leq$
 148 $\sup_{z \in \sigma(B)} |r(z)^{-1}|$. We conclude by the definition of $r(z)$ that

$$(6) \quad \frac{\sigma_{j+\nu k}(X)}{\sigma_j(X)} \leq \sup_{z \in \sigma(A)} |r(z)| \sup_{z \in \sigma(B)} \frac{1}{|r(z)|} = Z_k(\sigma(A), \sigma(B)) \leq Z_k(E, F),$$

150 as required. \square

151 Theorem 2.1 shows that if A and B are normal matrices in (1.1), then the singular
 152 values decay at least as fast as $Z_k(\sigma(A), \sigma(B))$ in (1.4). In particular, when $\sigma(A)$ and
 153 $\sigma(B)$ are disjoint and well-separated we expect $Z_k(\sigma(A), \sigma(B))$ to decay rapidly to
 154 zero and hence, so do the singular values of X .

155 For those readers that are familiar with the ADI method [13], an analogous proof
 156 of Theorem 2.1 is to run the ADI method for k steps with shift parameters given
 157 by the zeros and poles of the extremal rational function for $Z_k(E, F)$. By doing this

one constructs a rank νk approximant $X_{\nu k}$ for X , which shows that $\sigma_{1+\nu k}(X) \leq \|X - X_{\nu k}\|_2 \leq Z_k(E, F)\sigma_1(X)$. The connection between Zolotarev numbers and the optimal parameter selection for the ADI method has been previously exploited [27]. We have presented the above proof here because it does not require knowledge of the ADI method.

For matrices A and B that are not normal, Theorem 2.1 can be extended by using K -spectral sets [3]. Given a matrix A , a complex set E is said to be a K -spectral set for A if the spectrum $\sigma(A)$ of A is contained in E and the inequality $\|r(A)\|_2 \leq K\|r\|_E$ holds for every bounded rational function on E , where $\|r\|_E = \sup_{z \in E} |r(z)|$. Similar extensions have been noted when $B = A^*$ in (1.1) and the sets E and F are taken to be the fields of values for A and B , respectively [4]. We have the following extension of Theorem 2.1:

COROLLARY 2. *Suppose that the assumptions of Theorem 2.1 hold, except that the matrices A and B are not necessarily normal. Also suppose that E and F are K -spectral sets for A and B for some fixed constant $K > 0$, respectively. Then, we have $\sigma_{j+\nu k}(X) \leq K^2 Z_k(E, F)\sigma_j(X)$.*

Proof. It is only the first inequality in (2.2) of the proof of Theorem 2.1 that requires A and B to be normal matrices. When A is not a normal matrix, then the inequality $\|r(A)\|_2 \leq \sup_{z \in \sigma(A)} |r(z)|$ may not hold. Instead, we replace it by the K -spectral set bound given by $\|r(A)\|_2 \leq K\|r\|_E$. Note that since $p(z)$ and $q(x)$ are not zero on F and E , respectively, one can show via the Schur decomposition that $p(B)$ and $q(A)$ are invertible matrices. \square

Theorem 2.1 and Corollary 2.2 provide bounds on the singular values of X in terms of Zolotarev numbers. Therefore, to derive analytic bounds on the singular values of matrices with displacement structure, we must now calculate explicit bounds on Zolotarev numbers — a topic that fortunately is extensively studied.

3. Zolotarev numbers. In this section, we derive explicit lower and upper bounds for the Zolotarev numbers

$$Z_k := Z_k([-b, -a], [a, b]), \quad 0 < a < b < \infty,$$

which we use in Sections 4 and 5. The sharpest bounds that we are aware of in the literature take the form

$$(7) \quad \rho^{-2k} \leq Z_k \leq 16\rho^{-2k},$$

see [21, Theorem 1] for the lower bound, and [16, Eqn. (2.3)] for the upper bound.³ There are also bounds obtained directly from an infinite product formula for $\sqrt{Z_k}$ [27, (1.11)]; unfortunately, the original product formula in [27, (1.11)] contains typos and the erroneous formula has been copied elsewhere, for example, [24, (4.1)], [28, (3.17)], and [32, Sec. 4].⁴ We prove a corrected infinite product formula in Theorem 3.1 and further discuss the typos in Appendix A.

The value of ρ in (3.1) is related to the logarithmic capacity of a condenser with

³See also [15, Eqn. (A1)] and [10, proof of Thm. 6.6] for the related problem of minimal Blaschke products, and see [14, Theorem V.5.5] for how to deal with rational functions with different degree constraints.

⁴As one consequence of the erroneous formula in [27, (1.11)], a claimed lower bound in [28, (3.17)] and [27, (1.12)] is accidentally an upper bound. Unfortunately, the lower bound in [32, (15)] also appears to be in error. (See Appendix A for more details.)

plates $[-b, -a]$ and $[a, b]$:

$$(8) \quad \rho^2 = \exp\left(\frac{1}{\text{cap}([-b, -a], [a, b])}\right), \quad \rho = \exp\left(\frac{\pi^2}{2\mu(a/b)}\right),$$

where $\mu(\lambda) = \frac{\pi}{2}K(\sqrt{1-\lambda^2})/K(\lambda)$ is the Grötzsch ring function, and K is the complete elliptic integral of the first kind [31, (19.2.8)]

$$K(\lambda) = \int_0^1 \frac{1}{\sqrt{(1-t^2)(1-\lambda^2 t^2)}} dt, \quad 0 \leq \lambda \leq 1.$$

The bounds in (3.1) are not asymptotically sharp, and in Corollary 3.2 we show that the constant of “16” in the upper bound can be replaced by “4”. For a proof of this sharper upper bound, we first return to the work of Lebedev [27] and derive a corrected infinite product formula for Z_k .

THEOREM 3. *Let $k \geq 1$ be an integer and $0 < a < b < \infty$. Then for $Z_k := Z_k([-b, -a], [a, b])$ we have*

$$Z_k = 4\rho^{-2k} \prod_{\tau=1}^{\infty} \frac{(1 + \rho^{-8\tau k})^4}{(1 + \rho^{4k}\rho^{-8\tau k})^4}, \quad \rho = \exp\left(\frac{\pi^2}{2\mu(a/b)}\right),$$

where $\mu(\cdot)$ is the Grötzsch ring function.

Proof. We start by establishing a product formula for the inverse of μ that is apparently not widely known. For $\kappa \in (0, 1)$ set $q = \exp(-2\mu(\kappa))$. Since $\mu(\kappa) = \frac{\pi}{2}K(\sqrt{1-\kappa^2})/K(\kappa)$, we have that $q = \exp(-\pi K(\sqrt{1-\kappa^2})/K(\kappa))$ and from [31, (22.2.2)] we obtain

$$(9) \quad \kappa = \left(\frac{\theta_2(0, q)}{\theta_3(0, q)}\right)^2 = 4\sqrt{q} \prod_{\tau=1}^{\infty} \frac{(1 + q^{2\tau})^4}{(1 + q^{2\tau-1})^4}, \quad q = q(\kappa) = \exp(-2\mu(\kappa)).$$

Here, $\theta_2(z, q)$ and $\theta_3(z, q)$ are the classical theta functions [31, (20.2.2) & (20.2.3)] and the second equality above is derived from the infinite product formula in [31, (20.4.3) & (20.4.4)].

In order to deduce an explicit product formula for Z_k , we first note that the value of $2\sqrt{Z_k}/(1 + Z_k)$ is extensively reviewed by Akhiezer,⁵ see [1, Sec. 51], [1, Tab. 1 & 2, p. 150, No. 7 & 8], and [1, Tab. XXIII]. This value is equal to [1, p. 149], for some $\lambda_k \in (0, 1)$,

$$\frac{2\sqrt{Z_k}}{1 + Z_k} = \frac{1 - \lambda_k}{1 + \lambda_k}, \quad k\mu(\lambda_k) = \mu(a/b).$$

Here, there is a unique $\lambda_k \in (0, 1)$ since the Grötzsch ring function $\mu : [0, 1] \rightarrow [0, \infty]$ is a strictly decreasing bijection. Next, we recall that Gauss’ transformation [1, Tab. XXI] and Landen’s transformation [1, Tab. XX] are given by

$$(10) \quad \mu\left(\frac{2\sqrt{\lambda}}{1 + \lambda}\right) = \frac{\mu(\lambda)}{2}, \quad \mu\left(\frac{1 - \lambda}{1 + \lambda}\right) = 2\mu(\sqrt{1 - \lambda^2}), \quad \lambda \in (0, 1),$$

from which we conclude that

$$(11) \quad \mu(Z_k) = 2\mu\left(\frac{2\sqrt{Z_k}}{1 + Z_k}\right) = 4\mu\left(\sqrt{1 - \lambda_k^2}\right) = \frac{\pi^2}{\mu(\lambda_k)} = \frac{\pi^2 k}{\mu(a/b)}.$$

⁵There is a typo in [1, Tab. 1 & 2, p. 150, No. 7 & 8]. There should be no prime on λ_1 .

Therefore, from (3.5) we have

$$q = q(Z_k) = e^{-2\mu(Z_k)} = \exp\left(-2k \frac{\pi^2}{\mu(a/b)}\right) = \rho^{-4k},$$

where ρ is given in (3.2). The infinite product formula for Z_k follows by setting $\kappa = Z_k$ and $q = \rho^{-4k}$ in (3.3). \square

The infinite product in Theorem 3.1 can be estimated by observing that $(1 + \rho^{-4k} \rho^{-8\tau k})^2 \leq (1 + \rho^{-8\tau k})^2 \leq (1 + \rho^{-4k} \rho^{-8\tau k})(1 + \rho^{4k} \rho^{-8\tau k})$ for all $\tau \geq 1$. This leads to the following simple upper and lower bounds which are sufficient for the purpose of our paper.

COROLLARY 4. *Let $k \geq 1$ be an integer and $0 < a < b < \infty$. Then for $Z_k := Z_k([-b, -a], [a, b])$ we have*

$$\frac{4\rho^{-2k}}{(1 + \rho^{-4k})^4} \leq Z_k \leq \frac{4\rho^{-2k}}{(1 + \rho^{-4k})^2} \leq 4\rho^{-2k}, \quad \rho = \exp\left(\frac{\pi^2}{2\mu(a/b)}\right),$$

where $\mu(\cdot)$ is the Grötzsch ring function.

Corollary 3.2 shows that $Z_k \leq 4\rho^{-2k}$ is an asymptotically sharp upper bound in the sense that the geometric decay rate and the constant “4” cannot be improved if one hopes for the bound to hold for all k . However, this does not necessarily imply that our derived singular value inequalities are asymptotically sharp. On the contrary, they are usually not. For asymptotically sharp singular value bounds, we expect that one must consider discrete Zolotarev numbers, i.e., $Z_k(\sigma(A), \sigma(B))$ in Theorem 2.1, which are more subtle to bound and are outside the scope of this paper.

We often prefer the following slightly weaker bound that does not contain the Grötzsch ring function:

$$Z_k([-b, -a], [a, b]) \leq 4 \left[\exp\left(\frac{\pi^2}{2 \log(4b/a)}\right) \right]^{-2k}, \quad 0 < a < b < \infty,$$

which is obtained by using the bound $\mu(\lambda) \leq \log((2(1 + \sqrt{1 - \lambda^2}))/\lambda) \leq \log(4/\lambda)$, see [31, (19.9.5)]. This makes our final bounds on the singular values and ϵ -rank of matrices with displacement rank more intuitive to those readers that are less familiar with the Grötzsch ring function.

Later, in Section 5 we will need to use properties of an extremal rational function for $Z_k = Z_k([-b, -a], [a, b])$ and we prove them now. Zolotarev [45] studied the value Z_k and gave an explicit expression for the extremal function for Z_k (see (1.4)) by showing an equivalence to the problem of best rational approximation of the sign function on $[-b, -a] \cup [a, b]$. We now repeat this to derive the desired properties of the extremal rational function.

THEOREM 5. *Let $k \geq 1$ be an integer and $0 < a < b < \infty$. There exists an extremal function $R \in \mathcal{R}_{k,k}$ for $Z_k = Z_k([-b, -a], [a, b])$ such that*

- (a) *For $z \in [-b, -a]$, we have $-\sqrt{Z_k} \leq R(z) \leq \sqrt{Z_k}$,*
- (b) *For $z \in \mathbb{C}$, we have $R(-z) = 1/R(z)$, and*
- (c) *For $z \in \mathbb{R}$, we have $|R(iz)| = 1$.*

Proof. We give an explicit expression for an extremal function for Z_k by deriving it from the best rational approximation of the sign function on $[-b, -a] \cup [a, b]$. According to [1, Sec. 50 & 51, p. 144, line 6] we have

$$\inf_{r \in \mathcal{R}_{k,k}} \sup_{z \in [-b, -a] \cup [a, b]} |\operatorname{sgn}(z) - r(z)| = \frac{2\sqrt{Z_k}}{1 + Z_k}, \quad \operatorname{sgn}(z) = \begin{cases} 1, & z \in [a, b], \\ -1, & z \in [-b, -a], \end{cases}$$

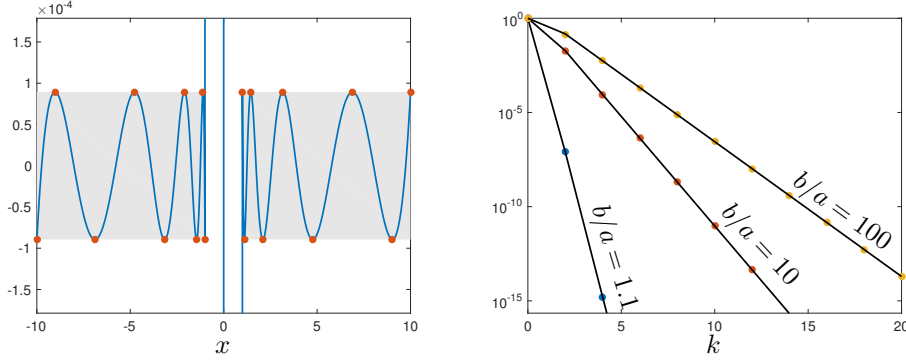


FIG. 1. Zolotarev's rational approximations. Left: The error between the sign function on $[-10, -1] \cup [1, 10]$ and its best rational $\mathcal{R}_{8,8}$ approximation on the domain $[-10, 10]$. The error equioscillates 9 times in the interval $[-10, -1]$ and $[1, 10]$ (see red dots), verifying its optimality [1, p. 149]. Right: The upper bound (black line) on $Z_k([-b, -a], [a, b])$ (colored dots) in Corollary 3.2 for $0 \leq k \leq 20$, with $b/a = 1.1$ (blue), 10 (red), 100 (yellow).

where the infimum is attained by the rational function [1, Sec. 51, Tab. 2, No. 7 & 8]

$$(12) \quad \tilde{r}(z) = Mz \frac{\prod_{j=1}^{\lfloor (k-1)/2 \rfloor} z^2 + c_{2j}}{\prod_{j=1}^{\lfloor k/2 \rfloor} z^2 + c_{2j-1}}, \quad c_j = a^2 \frac{\operatorname{sn}^2(jK(\kappa)/k; \kappa)}{1 - \operatorname{sn}^2(jK(\kappa)/k; \kappa)}.$$

Here, M is a real constant selected so that $\operatorname{sgn}(z) - \tilde{r}(z)$ equioscillates on $[-b, -a] \cup [a, b]$, $\kappa = \sqrt{1 - (a/b)^2}$, and $\operatorname{sn}(\cdot)$ is the first Jacobian elliptic function. Figure 3.1 (left) shows the error between the sign function on $[-10, -1] \cup [1, 10]$ and its best $\mathcal{R}_{8,8}$ rational approximation, which equioscillates 9 times on $[-10, -1]$ and $[1, 10]$ to confirm its optimality.

In order to construct an extremal function for Z_k with the required properties, we observe from (3.6) that M and c_1, \dots, c_{k-1} are real, and thus

- $\tilde{r}(z)$ is real-valued for $z \in \mathbb{R}$,
- $\tilde{r}(iz)$ is purely imaginary for $z \in \mathbb{R}$, and
- $\tilde{r}(z)$ is an odd function on \mathbb{R} , i.e., $\tilde{r}(z) = -\tilde{r}(-z)$ for $z \in \mathbb{R}$.

As a consequence, the rational function given by

$$R(z) = \frac{1 + \frac{1+Z_k}{1-Z_k} \tilde{r}(z)}{1 - \frac{1+Z_k}{1-Z_k} \tilde{r}(z)} \in \mathcal{R}_{k,k}$$

is real-valued for $z \in \mathbb{R}$ with $R(-z) = 1/R(z)$, and of modulus 1 on the imaginary axis. Finally, as $\tilde{r}(z)$ takes values in the interval

$$\left[-1 - \frac{2\sqrt{Z_k}}{1 + Z_k}, -1 + \frac{2\sqrt{Z_k}}{1 + Z_k} \right] = \left[\frac{-(1 + \sqrt{Z_k})^2}{1 + Z_k}, \frac{-(1 - \sqrt{Z_k})^2}{1 + Z_k} \right]$$

for $z \in [-b, -a]$, we have

$$\frac{1 + Z_k}{1 - Z_k} \tilde{r}(z) \in \left[-\frac{1 + \sqrt{Z_k}}{1 - \sqrt{Z_k}}, -\frac{1 - \sqrt{Z_k}}{1 + \sqrt{Z_k}} \right],$$

implying that $-\sqrt{Z_k} \leq R(z) \leq \sqrt{Z_k}$ for $z \in [-b, -a]$. Hence, using $R(-z) = 1/R(z)$ we have

$$\frac{\sup_{z \in E} |R(z)|}{\inf_{z \in F} |R(z)|} \leq Z_k = \inf_{r \in \mathcal{R}_{k,k}} \frac{\sup_{z \in E} |r(z)|}{\inf_{z \in F} |r(z)|},$$

showing that R is extremal for $Z_k([-b, -a], [a, b])$, as required. \square

Figure 3.1 (right) demonstrates the upper bound in Corollary 3.2 when $b/a = 1.1, 10, 100$. In Section 4 we combine our upper bound on the singular values in Theorem 2.1 with our upper bound on Zolotarev numbers to derive explicit bounds on the singular values of certain Pick, Cauchy, and Löwner matrices.

4. The decay of the singular values of Pick, Cauchy, and Löwner matrices. In this section we bound the singular values of Pick (see Section 4.1), Cauchy (see Section 4.2), and Löwner (see Section 4.3) matrices. In view of Theorem 2.1 and Corollary 3.2, our first idea is to construct matrices A and B so that the rank of $AX - XB$ is small with the additional hope that $\sigma(A)$ and $\sigma(B)$ are contained in real and disjoint intervals. For the three classes of matrices in this section, this first idea works out under mild “separation conditions”. In Section 5 the more challenging cases of Krylov, real Vandermonde, and real positive definite Hankel matrices are considered.

4.1. Pick matrices. An $n \times n$ matrix P_n is called a Pick matrix if there exists a vector $\underline{s} = (s_1, \dots, s_n)^T \in \mathbb{C}^{n \times 1}$, and a collection of real numbers $x_1 < \dots < x_n$ from an interval $[a, b]$ with $0 < a < b < \infty$ such that

$$(P_n)_{jk} = \frac{s_j + s_k}{x_j + x_k}, \quad 1 \leq j, k \leq n.$$

All Pick matrices satisfy the following Sylvester matrix equation:

$$D_{\underline{x}} P_n - P_n (-D_{\underline{x}}) = \underline{s} \underline{e}^T + \underline{e} \underline{s}^T, \quad D_{\underline{x}} = \text{diag}(x_1, \dots, x_n),$$

where $\underline{e} = (1, \dots, 1)^T$. Since diagonal matrices are normal matrices and in this case the spectrum of $D_{\underline{x}}$ is contained in $[a, b]$, we have the following bounds on the singular values of P_n .

COROLLARY 6. *Let P_n be the $n \times n$ Pick matrix in (4.1). Then, for $j \geq 1$ we have*

$$\sigma_{j+2k}(P_n) \leq 4 \left[\exp \left(\frac{\pi^2}{2\mu(a/b)} \right) \right]^{-2k} \sigma_j(P_n), \quad 1 \leq j + 2k \leq n,$$

where $\mu(\lambda)$ is the Grötzsch ring function (see Section 3). The bound remains valid, but is slightly weaker, if $\mu(a/b)$ is replaced by $\log(4b/a)$.

Proof. From (4.2), we know that $A = D_{\underline{x}}$, $B = -A$, $\nu = 2$, $E = [a, b]$, and $F = [-b, -a]$ in Theorem 2.1. Therefore, for $j \geq 1$ we have $\sigma_{j+2k}(P_n) \leq Z_k(E, F) \sigma_j(P_n)$, $1 \leq j + 2k \leq n$. The result follows from the upper bound in Corollary 3.2. \square

There are two important consequences of Corollary 4.1: (1) Pick matrices are usually ill-conditioned unless b/a is large and/or n is small and (2) All Pick matrices can be approximated, up to an accuracy of $\epsilon \|X\|_2$ with $0 < \epsilon < 1$, by a rank $\mathcal{O}(\log(b/a) \log(1/\epsilon))$ matrix. More precisely, for any Pick matrix in (4.1) we have

$$\kappa_2(P_n) = \frac{\sigma_1(P_n)}{\sigma_n(P_n)} \geq \frac{1}{4} \left[\exp \left(\frac{\pi^2}{2 \log(4b/a)} \right) \right]^{2 \lceil \frac{n}{2} - 1 \rceil},$$

where for an even integer n we used $\sigma_1(P_n)/\sigma_n(P_n) \geq \sigma_1(P_n)/\sigma_{n-1}(P_n)$. Moreover, by setting k to be the smallest integer so that $\sigma_{1+2k}(P_n) \leq \epsilon \sigma_1(P_n)$, we find the following bound on the ϵ -rank of P_n (see (1.3)):

$$\text{rank}_\epsilon(P_n) \leq 2 \left\lceil \frac{\log(4b/a) \log(4/\epsilon)}{\pi^2} \right\rceil.$$

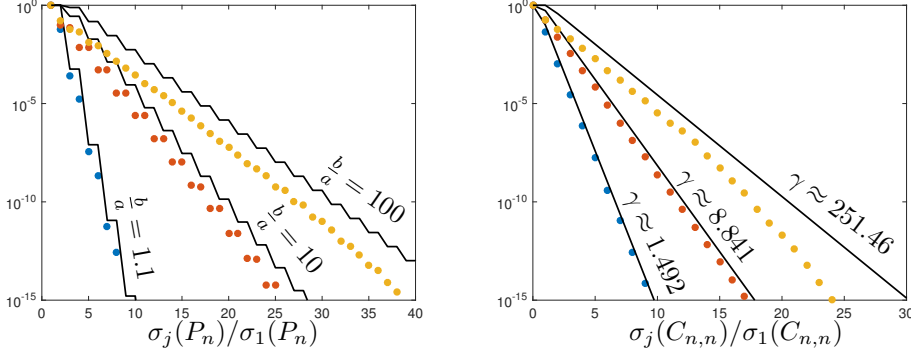


FIG. 2. Left: The scaled singular values of 100×100 Pick matrices (colored dots) and the bound in Corollary 4.1 (black line) for $b/a = 1.1$ (blue), 10 (red), 100 (yellow). In (4.1), \underline{x} is a vector of equally spaced points in $[a, b]$ and \underline{s} is a random vector with independent standard Gaussian entries. Right: The scaled singular values of 100×100 Cauchy matrices (colored dots) and the bound in Corollary 4.2 (black line) for $\gamma = 1.1, 10, 100$. In (4.5), \underline{x} is a vector of Chebyshev nodes from $[-8.5, -2]$ (blue), $[-100, -3]$ (red), and $[-101, 2.8]$ (yellow), respectively, \underline{y} is a vector of Chebyshev nodes from $[3, 10]$ (blue), $[3, 100]$ (red), and $[3, 100]$ (yellow), respectively, and \underline{s} and \underline{t} are random vectors with independent standard Gaussian entries. The decay rate depends on the cross-ratio of the endpoints of the intervals.

In both (4.3) and (4.4), the bound can be slightly improved by replacing the $\log(4b/a)$ term by $\mu(a/b)$. Previously, bounds on the minimum and maximum singular values of Pick matrices were derived under the additional assumption that P_n is a positive definite matrix [18].

Figure 4.1 (left) demonstrates the bound in Corollary 4.1 on three 100×100 Pick matrices. The black line bounding the singular values has a stepping behavior because the inequality in Corollary 4.1 for $j = 1$ only bounds odd indexed singular values of P_n and to bound $\sigma_{2k}(P_n)$ we use the trivial inequality $\sigma_{2k}(P_n) \leq \sigma_{2k-1}(P_n)$. At this time we can offer little insight into why the singular values of the tested Pick matrices also have a similar stepping behavior.

4.2. Cauchy matrices. An $m \times n$ matrix $C_{m,n}$ with $m \geq n$ is called a (generalized) Cauchy matrix if there exists vectors $\underline{s} \in \mathbb{C}^{m \times 1}$ and $\underline{t} \in \mathbb{C}^{n \times 1}$, points $x_1 < \dots < x_m$ on an interval $[a, b]$ with $-\infty < a < b < \infty$, and points $y_1 < \dots < y_n$ (all distinct from x_1, \dots, x_m) in an interval $[c, d]$ with $-\infty < c < d < \infty$ such that

$$(C_{m,n})_{jk} = \frac{s_j t_k}{x_j - y_k}, \quad 1 \leq j \leq m, \quad 1 \leq k \leq n. \quad (17)$$

Generalized Cauchy matrices satisfy the following Sylvester matrix equation:

$$D_{\underline{x}} C_{m,n} - C_{m,n} D_{\underline{y}} = \underline{s} \underline{t}^T, \quad (18)$$

where $D_{\underline{x}} = \text{diag}(x_1, \dots, x_m)$ and $D_{\underline{y}} = \text{diag}(y_1, \dots, y_n)$.

If we make the further assumption that either $b < c$ or $d < a$ so that the intervals $[a, b]$ and $[c, d]$ are disjoint, then we can bound the singular values of $C_{m,n}$. This “separation condition” is an extra assumption on Cauchy matrices that simplifies the analysis. If the intervals $[a, b]$ and $[c, d]$ overlapped, then one would have to consider discrete Zolotarev numbers to estimate the singular values and we want to avoid this in this paper.

COROLLARY 7. Let $C_{m,n}$ be an $m \times n$ Cauchy matrix in (4.5) with $m \geq n$ and either $b < c$ or $d < a$. Then,

$$\sigma_{j+k}(C_{m,n}) \leq 4 \left[\exp \left(\frac{\pi^2}{4\mu(1/\sqrt{\gamma})} \right) \right]^{-2k} \sigma_j(C_{m,n}), \quad 1 \leq j+k \leq n,$$

where γ is the absolute value of the cross-ratio⁶ of a, b, c , and d . If $a = c$ and $b = d$, then $2\mu(1/\sqrt{\gamma}) = \mu(a/b)$. The bound remains valid, but is slightly weakened, if $4\mu(1/\sqrt{\gamma})$ is replaced by $2\log(16\gamma)$.

Proof. From (4.6), we know that $A = D_{\underline{x}}$, $B = D_{\underline{y}}$, $\nu = 1$, $E = [a, b]$, and $F = [c, d]$ in Theorem 2.1. Therefore, we conclude that $\sigma_{j+k}(C_{m,n}) \leq Z_k(E, F)\sigma_j(C_{m,n})$ for $1 \leq j+k \leq n$.

The value of $Z_k(E, F)$ is invariant under Möbius transformations. That is, if $T(z) = (a_1z + a_2)/(a_3z + a_4)$ is a Möbius transformation, then $Z_k(E, F)$ and $Z_k(T(E), T(F))$ are equal. Therefore, we can transplant $[a, b] \cup [c, d]$ onto $[-\alpha, -1] \cup [1, \alpha]$ for some $\alpha > 1$ using a Möbius transformation. If $b < c$, then the transformation satisfies $T(a) = -\alpha$, $T(b) = -1$, $T(c) = 1$, $T(d) = \alpha$. Since T is a Möbius transformation the cross-ratio of the four collinear points a, b, c , and d equals the cross-ratio of $T(a), T(b), T(c)$, and $T(d)$. Hence, if $b < c$ or $d < a$ then we know that α must satisfy

$$\frac{|c-a||d-b|}{|c-b||d-a|} = \frac{(\alpha+1)^2}{4\alpha}.$$

Therefore, by solving the quadratic and noting that $\alpha > 1$ we have

$$(19) \quad \alpha = -1 + 2\gamma + 2\sqrt{\gamma^2 - \gamma}, \quad \gamma = \frac{|c-a||d-b|}{|c-b||d-a|}.$$

From Corollary 3.2, we conclude that

$$\sigma_{j+k}(C_{m,n}) \leq 4 \left[\exp \left(\frac{\pi^2}{2\mu(1/\alpha)} \right) \right]^{-2k} \sigma_j(C_{m,n}), \quad 1 \leq j+k \leq n.$$

By Gauss' transformation in (3.4), we note that $\mu(1/\alpha) = 2\mu(1/\sqrt{\gamma}) \leq 2\log(4\sqrt{\gamma}) = \log(16\gamma)$ and the result follows. \square

It is interesting to observe that the decay rate of the singular values of Cauchy matrices only depends on the absolute value of the cross-ratio of a, b, c , and d . Hence, the "separation" of two real intervals $[a, b]$ and $[c, d]$ for the purposes of singular value estimates is measured in terms of the cross-ratio of a, b, c , and d , not the separation distance $\max(c-b, a-d)$.

Corollary 4.2 shows that the Cauchy matrix in (4.5) (when $b < c$ or $d < a$) has an ϵ -rank of at most

$$\text{rank}_\epsilon(C_{m,n}) \leq \left\lceil \frac{2\mu(1/\sqrt{\gamma})\log(4/\epsilon)}{\pi^2} \right\rceil \leq \left\lceil \frac{\log(16\gamma)\log(4/\epsilon)}{\pi^2} \right\rceil,$$

where γ is absolute value of the cross-ratio of a, b, c , and d . Bounds on the numerical rank of the Cauchy matrix have also been obtained via the Cauchy function, i.e., $1/(x+y)$ on $[a, b] \times [c, d]$, by exploiting the hierarchical low rank structure of $C_{m,n}$ [22]

⁶Given four collinear points a, b, c , and d the cross-ratio is given by $(c-a)(d-b)/((c-b)(d-a))$.

(for more details, see [39, Chapter 3]). Furthermore, when $m = n$ (and $b < c$ or $d < a$) we have a lower bound on the condition number of $C_{n,n}$:

$$\kappa_2(C_{n,n}) = \frac{\sigma_1(C_{n,n})}{\sigma_n(C_{n,n})} \geq \frac{1}{4} \left[\exp \left(\frac{\pi^2}{2 \log(16\gamma)} \right) \right]^{2(n-1)}, \quad \gamma = \frac{|c-a||d-b|}{|c-b||d-a|}.$$

Corollary 4.2 also includes the important Hilbert matrix, i.e., $(H_n)_{jk} = 1/(j+k-1)$ for $1 \leq j, k \leq n$. By setting $x_j = j - 1/2$, $y_j = -k + 1/2$, and $\underline{s} = \underline{r} = (1, \dots, 1)^T$, the matrix in (4.5) is the Hilbert matrix. In particular, Corollary 4.2 with $[a, b] = [-n + 1/2, -1/2]$ and $[c, d] = [1/2, n - 1/2]$ shows that

$$(20) \quad \sigma_{k+1}(H_n) \leq 4 \left[\exp \left(\frac{\pi^2}{2 \log(8n-4)} \right) \right]^{-2k} \sigma_1(H_n), \quad 1 \leq k \leq n-1.$$

Therefore, the Hilbert matrix can be well-approximated by a low rank matrix and has exponentially decaying singular values.⁷ In particular, it has an ϵ -rank of at most $\lceil \log(8n-4) \log(4/\epsilon)/\pi^2 \rceil$. The Hilbert matrix is an example of a real positive definite Hankel matrix and in Section 5 we show that bounds similar to (4.8) hold for the singular values of all such matrices.

Figure 4.1 (right) demonstrates the bound in Corollary 4.2 on three $n \times n$ Cauchy matrices, where $n = 100$. In practice, the derived bound is relatively tight for singular values $\sigma_j(C_{m,n})$ when j is small with respect to n .

4.3. Löwner matrices. An $n \times n$ matrix L_n is called a Löwner matrix if there exist vectors $\underline{r}, \underline{s} \in \mathbb{C}^{n \times 1}$, points $x_1 < \dots < x_n$ in $[a, b]$ with $-\infty < a < b < \infty$, and points $y_1 < \dots < y_n$ (all different from x_1, \dots, x_n) in $[c, d]$ with $-\infty < c < d < \infty$ such that

$$(21) \quad (L_n)_{jk} = \frac{r_j - s_k}{x_j - y_k}, \quad 1 \leq j, k \leq N.$$

In the special case when $y_j = -x_j$ and $s_j = -r_j$, a Löwner matrix is a Pick matrix (see Section 4.1). Löwner matrices satisfy the Sylvester matrix equation given by

$$D_{\underline{x}} L_n - L_n D_{\underline{y}} = \underline{r} \underline{e}^T - \underline{e} \underline{s}^T,$$

where $\underline{e} = (1, \dots, 1)^T$. From Theorem 2.1 we can bound the singular values of L_n provided that $[a, b]$ and $[c, d]$ are disjoint, i.e., either $b < c$ or $d < a$. We emphasize that the separation condition of the intervals $[a, b]$ and $[c, d]$ is an extra assumption on a Löwner matrix that allows us to proceed with the methodology we have developed.

COROLLARY 8. *Let L_n be an $n \times n$ Löwner matrix in (4.9) with $b < c$ or $d < a$. Then, for $j \geq 1$ we have*

$$\sigma_{j+2k}(L_n) \leq 4 \left[\exp \left(\frac{\pi^2}{4\mu(1/\sqrt{\gamma})} \right) \right]^{-2k} \sigma_j(L_n), \quad 1 \leq j + 2k \leq n,$$

where γ is the absolute value of the cross-ratio of a, b, c , and d (see (4.7)). If $a = c$ and $b = d$, then $2\mu(1/\sqrt{\gamma}) = \mu(a/b)$. The bound remains valid, but is slightly weakened, if $4\mu(1/\sqrt{\gamma})$ is replaced by $2\log(16\gamma)$.

⁷More generally, skeleton decompositions can be used to show that the Hilbert kernel of $f(x, y) = 1/(x+y)$ on $[a, b] \times [a, b]$ with $0 < a < b < \infty$ has exponentially decaying singular values [32]. Even though there is an error in [32, Sec. 4] in the infinite product formula and the stated lower bound (see Appendix A), we believe the proved upper bound in [32, (15)] is correct.

Proof. The same argument as in Corollary 4.2, but with $\nu = 2$. \square
 Corollary 4.3 shows that many Löwner matrices can be well-approximated by low rank matrices with $\text{rank}_\epsilon(L_n) = \mathcal{O}(\log \gamma \log(1/\epsilon))$ and are exponentially ill-conditioned.

5. The singular values of Krylov, Vandermonde, and Hankel matrices.

The three types of matrices considered in Section 4 allowed for direct applications of Theorem 2.1 and Corollary 3.2. In this section, we consider the more challenging tasks of bounding the singular values of Krylov matrices with Hermitian arguments, real Vandermonde matrices, and real positive definite Hankel matrices.

5.1. Krylov and real Vandermonde matrices. An $m \times n$ matrix $K_{m,n}$ with $m \geq n$ is said to be a Krylov matrix with Hermitian argument if there exists a Hermitian matrix $A \in \mathbb{C}^{m \times m}$ and a vector $\underline{w} \in \mathbb{C}^{m \times 1}$ such that

$$(22) \quad K_{m,n} = \begin{bmatrix} \underline{w} & A\underline{w} & \cdots & A^{n-1}\underline{w} \end{bmatrix}.$$

Vandermonde matrices of size $m \times n$ with real abscissas $\underline{x} \in \mathbb{R}^{m \times 1}$, i.e., $(V_{m,n})_{jk} = x_j^{k-1}$, are also Krylov matrices with $A = D_{\underline{x}}$ and $\underline{w} = (1, \dots, 1)^T$. Krylov matrices satisfy the following Sylvester matrix equation:

$$(23) \quad AK_{m,n} - K_{m,n}Q = \underline{s}\underline{e}_n^T, \quad Q = \begin{bmatrix} 0 & & & -1 \\ 1 & & & \\ & \ddots & & \\ & & 1 & 0 \end{bmatrix},$$

where $\underline{s} \in \mathbb{C}^{m \times 1}$ and $\underline{e}_n = (0, \dots, 0, 1)^T$. Since A is a normal matrix, we attempt to use Theorem 2.1 to bound the singular values of $K_{m,n}$.

For the analysis that follows, we require that n is an even integer. This is not a loss of generality because by the interlacing theorem for singular values [38]. To see this, let $K_{m,n-1}$ be the $m \times (n-1)$ Krylov matrix obtained from $K_{m,n}$ by removing its last column. If n is odd, then⁸

$$(24) \quad \frac{\sigma_{j+k}(K_{m,n})}{\sigma_j(K_{m,n})} \leq \frac{\sigma_{j+k-1}(K_{m,n-1})}{\sigma_j(K_{m,n-1})}, \quad 2 \leq j+k \leq n,$$

and one can bound $\sigma_{j+k-1}(K_{m,n-1})/\sigma_j(K_{m,n-1})$ instead. From now on in this section we will assume that n is an even integer.

The Sylvester matrix equation in (5.2) contains matrices A and Q , which are both normal matrices. The eigenvalues of A are contained in \mathbb{R} and the eigenvalues of Q are the n (shifted) roots of unity, i.e.,

$$(25) \quad \sigma(Q) = \left\{ z \in \mathbb{C} : z = e^{\frac{2\pi i(j+1/2)}{n}}, 0 \leq j \leq n-1 \right\}.$$

Since n is even, the spectrum of Q and the real line are disjoint. Using Theorem 2.1 we find that for $j \geq 1$ and $1 \leq j+k \leq n$

$$(26) \quad \sigma_{j+k}(K_{m,n}) \leq Z_k(E, F)\sigma_j(K_{m,n}), \quad E \subseteq \mathbb{R}, \quad F = F_+ \cup F_-,$$

⁸Observe that the singular values of a matrix decrease when removing a column and thus $\sigma_j(K_{m,n-1}) \leq \sigma_j(K_{m,n})$. Let Y be a best rank $j+k-2$ approximation to $K_{m,n-1}$ so that $\sigma_{j+k-1}(K_{m,n-1}) = \|K_{m,n-1} - Y\|_2$ and consider X obtained from Y by concatenating (on the right) the last column of $K_{m,n}$. Then, the rank of X is at most $j+k-1$ and hence, $\sigma_{j+k}(K_{m,n}) \leq \|K_{m,n} - X\|_2 = \|K_{m,n-1} - Y\|_2 = \sigma_{j+k-1}(K_{m,n-1})$.

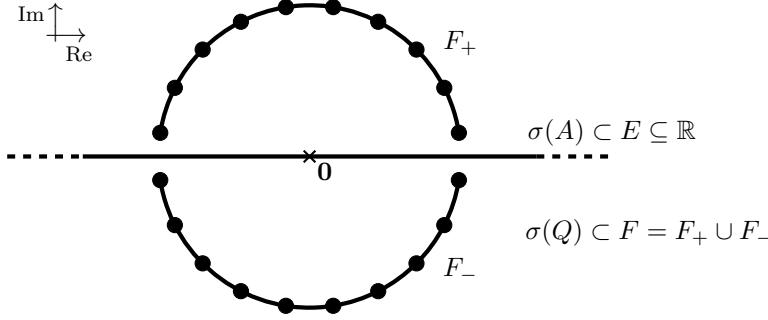


FIG. 3. The sets E and F in the complex plane for the Zolotarev problem (1.4) used to bound the singular values of a 20×20 Krylov matrix with a Hermitian argument. The sets F_+ and F_- are a distance of only $\mathcal{O}(1/n)$ from the real axis, where n is the size of the Krylov matrix, and this causes the $\log n$ dependence in the weakened version of (5.5). The solid black dots denote the spectrum of Q , which is contained in $F_+ \cup F_-$.

where F_+ and F_- are complex sets defined by

$$(25) \quad F_+ = \{e^{it} : t \in [\frac{\pi}{n}, \pi - \frac{\pi}{n}]\}, \quad F_- = \{e^{it} : t \in [-\pi + \frac{\pi}{n}, -\frac{\pi}{n}]\}.$$

Figure 5.1 shows the two sets E and F in the complex plane. As $n \rightarrow \infty$ the sets F_+ and F_- approach the real line, suggesting that our bound on the singular values must depend on n somehow. Our task is to bound the quantity $Z_k(E, F_+ \cup F_-)$ — a Zolotarev number that is not immediately related to one of the form $Z_k([-b, -a], [a, b])$.

The following lemma relates the quantity $Z_{2k}(E, F_+ \cup F_-)$ to the Zolotarev number $Z_k([-1/\ell, -\ell], [\ell, 1/\ell])$ with $\ell = \tan(\pi/(2n))$:

LEMMA 9. Let $k \geq 1$ be an integer and $E \subseteq \mathbb{R}$. Then, $Z_{2k+1}(E, F_+ \cup F_-) \leq Z_{2k}(E, F_+ \cup F_-)$ and

$$Z_{2k}(E, F_+ \cup F_-) \leq \frac{2\sqrt{Z_k}}{1 + Z_k}, \quad Z_k := Z_k([-1/\ell, -\ell], [\ell, 1/\ell]),$$

where $\ell = \tan(\pi/(2n))$, the complex sets F_+ and F_- are defined in (5.4), and n is an even integer.

Proof. Let $R(z) \in \mathcal{R}_{k,k}$ be the extremal function for $Z_k := Z_k([-1/\ell, -\ell], [\ell, 1/\ell])$ characterized in Theorem 3.3, where $\ell = \tan(\pi/(2n))$. Since the Möbius transform given by

$$T(z) = \frac{1}{i} \frac{z - 1}{z + 1}$$

maps F_+ to $[\ell, 1/\ell]$, F_- to $[-1/\ell, -\ell]$, and \mathbb{R} to $i\mathbb{R}$, we have

$$Z_{2k}(\mathbb{R}, F_+ \cup F_-) = Z_{2k}(i\mathbb{R}, [-1/\ell, -\ell] \cup [\ell, 1/\ell]) = \inf_{r \in \mathcal{R}_{2k,2k}} \frac{\sup_{z \in \mathbb{R}} |r(iz)|}{\inf_{z \in [-1/\ell, -\ell] \cup [\ell, 1/\ell]} |r(z)|}.$$

Now, consider the rational function

$$S(z) = \frac{R(z) + 1/R(z)}{2} = \frac{R(z) + R(-z)}{2} \in \mathcal{R}_{2k,2k},$$

where we used the fact that $1/R(z) = R(-z)$ (see Theorem 3.3, (b)). Since $|R(iz)| = 1$ for $z \in \mathbb{R}$ (see Theorem 3.3, (c)), we have

$$\sup_{z \in \mathbb{R}} |S(iz)| = \sup_{z \in \mathbb{R}} \left| \frac{R(iz) + R(-iz)}{2} \right| \leq 1.$$

Moreover, since $-1 \leq -\sqrt{Z_k} \leq R(z) \leq \sqrt{Z_k} \leq 1$ for $z \in [-1/\ell, -\ell]$ (see Theorem 3.3, (a)) and $x \mapsto 2x/(1+x^2)$ is a nondecreasing function on $[-1, 1]$ and $S(-z) = S(z)$, we have

$$\begin{aligned} \inf_{z \in [-1/\ell, -\ell] \cup [\ell, 1/\ell]} |S(z)| &= \sup_{z \in [-1/\ell, -\ell]} \left| \frac{2}{R(z) + 1/R(z)} \right| \\ &= \sup_{z \in [-1/\ell, -\ell]} \left| \frac{2R(z)}{1 + R(z)^2} \right| \\ &\leq \frac{2\sqrt{Z_k}}{1 + Z_k}. \end{aligned}$$

Therefore, $Z_{2k}(E, F_+ \cup F_-) \leq Z_{2k}(\mathbb{R}, F_+ \cup F_-) \leq 2\sqrt{Z_k}/(1 + Z_k)$ as required. The bound $Z_{2k+1}(E, F_+ \cup F_-) \leq Z_{2k}(E, F_+ \cup F_-)$ trivially holds from the definition of Zolotarev numbers. \square

By Corollary 3.2 we have the slightly weaker upper bound for $Z_{2k}(E, F_+ \cup F_-)$:

$$Z_{2k}(E, F_+ \cup F_-) \leq 2\sqrt{Z_k([-1/\ell, -\ell], [\ell, 1/\ell])} \leq 4\rho^{-k},$$

where since $\tan x \geq x$ for $0 \leq x \leq \pi/2$, we have

$$\rho = \exp\left(\frac{\pi^2}{2\mu(\tan(\pi/(2n))^2)}\right) \geq \exp\left(\frac{\pi^2}{2\log(4/\tan(\pi/(2n))^2)}\right) \geq \exp\left(\frac{\pi^2}{4\log(4n/\pi)}\right).$$

If n is an even integer, then we can immediately conclude a bound on the singular values from Theorem 2.1. If n is an odd integer, then one must employ (5.3) first.

COROLLARY 10. *The singular values of $K_{m,n}$ can be bounded as follows:*

$$(26) \quad \sigma_{j+2k}(K_{m,n}) \leq 4 \left[\exp\left(\frac{\pi^2}{2\mu(\tan(\pi/(4\lfloor n/2 \rfloor))^2)}\right) \right]^{-k+[n]_2} \sigma_j(K_{m,n}), \quad 1 \leq j+2k \leq n,$$

where $\mu(\cdot)$ is the Grötzsch function and $[n]_2 = 1$ if n is odd and is 0 if n is even. The bound above remains valid, but is slightly weaker, if $2\mu(\tan(\pi/(4\lfloor n/2 \rfloor))^2)$ is replaced by $4\log(8\lfloor n/2 \rfloor/\pi)$.

Figure 5.2 demonstrates the bound on the singular values in (5.5) on $n \times n$ Krylov matrices, where $n = 10, 100, 1000$. The step behavior of the bound is due to the fact that (5.5) only bounds $\sigma_{1+2k}(K_{m,n})$ when n is even and we use the trivial inequality $\sigma_{2k+2}(K_{m,n}) \leq \sigma_{2k+1}(K_{m,n})$ otherwise. One also observes that the singular values of Krylov matrices with Hermitian arguments can decay at a supergeometric rate; however, the analysis in this paper only realizes a geometric decay. Therefore, (5.5) is only a reasonable bound on $\sigma_j(K_{m,n})$ when j is a small integer with respect to n . If $j/n \rightarrow c$ and $c \in (0, 1)$, then improved bounds on $\sigma_j(K_{m,n})$ may be possible by bounding discrete Zolotarev numbers [9]. The bound in (5.5) provides an upper bound on the ϵ -rank of $K_{m,n}$:

$$\text{rank}_\epsilon(K_{m,n}) \leq 2 \left\lceil \frac{4\log(8\lfloor n/2 \rfloor/\pi) \log(4/\epsilon)}{\pi^2} \right\rceil + 2,$$

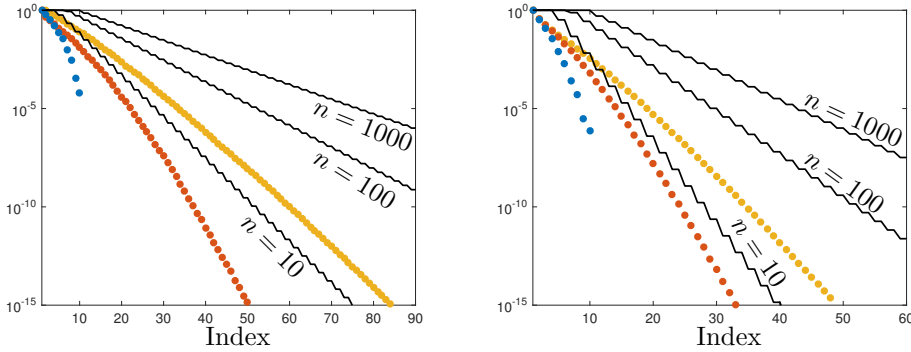


FIG. 4. Left: The singular values of $n \times n$ Krylov matrix (colored dots) compared to the bound in (5.5) for $n = 10$ (blue), 100 (red), 1000 (yellow). In (5.1) the matrix A is a diagonal matrix with entries taken to be equally spaced points in $[-1, 1]$ and \underline{w} is a random vector with independent Gaussian entries. Right: The singular values of the $n \times n$ real positive definite Hankel matrices (colored dots) associated to the measure $\mu_H(x) = \mathbf{1}_{[-1, 1]}$ compared to the bound in (5.7) for $n = 10$ (blue), 100 (red), 1000 (yellow).

which allows for either an odd or even integer n .

Recall that Vandermonde matrices with real abscissas are also Krylov matrices with Hermitian arguments. Therefore, the bounds in this section also apply to Vandermonde matrices with real abscissas and shows that they have rapidly decaying singular values and are exponentially ill-conditioned. An observation that has been extensively investigated in the literature [6, 20, 33].

5.2. Real positive definite Hankel matrices. An $n \times n$ matrix H_n is a Hankel matrix if the matrix is constant along each anti-diagonal, i.e., $(H_n)_{jk} = h_{j+k}$ for $1 \leq j, k \leq n$. Clearly, not all Hankel matrices have decaying singular values, for example, the exchange matrix has repeated singular values of 1. This means that any displacement structure that is satisfied by all Hankel matrices, for example,

$$\text{rank}(QX - XQ^T) \leq 2,$$

where Q is given in (5.2), does not result in a Zolotarev number that decays. Motivated by the Hilbert matrix in Section 4.2, we show that every real and positive definite Hankel matrix has rapidly decaying singular values. Previous work has led to bounds that can be calculated by using a pivoted Cholesky algorithm [2], bounds for very special cases [40], as well as incomplete attempts [41, 42].

In order to exploit the positive definite structure we recall that the Hamburger moment problem states that a real Hankel matrix is positive semidefinite if and only if it is associated to a nonnegative Borel measure supported on the real line.

LEMMA 11. A real $n \times n$ Hankel matrix, H_n , is positive semidefinite if and only if there exists a nonnegative Borel measure μ_H supported on the real line such that

$$(H_n)_{jk} = \int_{-\infty}^{\infty} x^{j+k-2} d\mu_H(x), \quad 1 \leq j, k \leq n.$$

Proof. For a proof, see [34, Theorem 7.1]. \square

Let H_n be a real positive definite Hankel matrix associated to the nonnegative weight μ_H in (5.6) supported on \mathbb{R} . Let x_1, \dots, x_n and w_1^2, \dots, w_n^2 be the Gauss quadrature nodes and weights associated to μ_H . Then, since a Gauss quadrature is

exact for polynomials of degree $2n - 1$ or less, we have

$$(H_n)_{jk} = \int_{-\infty}^{\infty} x^{j+k-2} d\mu_H(x) = \sum_{s=1}^n w_s^2 x_s^{j+k-2} = \sum_{s=1}^n (w_s x_s^{j-1})(w_s x_s^{k-1}).$$

Therefore, every real positive definite Hankel matrices has a so-called *Fiedler factorization* [19], i.e.,

$$H_n = K_{n,n}^* K_{n,n}, \quad K_{n,n} = \begin{bmatrix} \underline{w} & D_{\underline{x}} \underline{w} & \cdots & D_{\underline{x}}^{n-1} \underline{w} \end{bmatrix},$$

where $K_{n,n}$ is a Krylov matrix with Hermitian argument and $K_{n,n}^*$ is the conjugate transpose of $K_{n,n}$. This means that $\sigma_j(H_n) = \sigma_j(K_{n,n})^2$ for $1 \leq j \leq n$. That is, a bound on the singular values of H_n and the ϵ -rank of H_n directly follows from (5.5).

COROLLARY 12. *Let H_n be an $n \times n$ real positive definite Hankel matrix. Then,*

$$(28) \quad \sigma_{j+2k}(H_n) \leq 16 \left[\exp \left(\frac{\pi^2}{4 \log(8 \lfloor n/2 \rfloor / \pi)} \right) \right]^{-2k+2} \sigma_j(H_n), \quad 1 \leq j + 2k \leq n,$$

and

$$\text{rank}_{\epsilon}(H_n) \leq 2 \left\lceil \frac{2 \log(8 \lfloor n/2 \rfloor / \pi) \log(16/\epsilon)}{\pi^2} \right\rceil + 2,$$

where both bounds allow for n to be an even or odd integer.

We conclude that all real positive definite Hankel matrices have an ϵ -rank of at most $\mathcal{O}(\log n \log(1/\epsilon))$, explaining why low rank techniques are usually advantageous in computational mathematics on such matrices.

Since a real positive semidefinite Hankel matrix can be arbitrarily approximated by a real positive definite Hankel matrix, the results from this section immediately extend to such Hankel matrices.⁹ This fact was exploited, but not proved in general, in [40] to derive quasi-optimal complexity fast transforms between orthogonal polynomial bases.

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⁹For a real positive semidefinite Hankel matrix one may improve our bounds on the singular values of H_n by replacing n by the rank of H_n .

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Appendix A. Typos in an infinite product formula. In Section 3 we noted that there were typos in an infinite product formula given by Lebedev [27, (1.11)]. The mistake has unfortunately been copied several times in the literature. Here, we attempt to correct these typos.

Lebedev [27] and his successors [28, 32] were not concerned with the Zolotarev problem in (1.4), but instead the equivalent problem of minimal Blaschke products in the half plane, i.e.,

$$(29) \quad E_k([a, b]) = \min_{z_1, \dots, z_k \in \mathbb{C}} \max_{z \in [a, b]} \left| \prod_{s=1}^k \frac{z - z_s}{z + \bar{z}_s} \right|, \quad 0 < a < b < \infty.$$

In [27, (1.11)], Lebedev presented an infinite product formula for E_k that unfortunately contained typos and resulted in an erroneous lower bound for E_k in [27, (1.12)]. More recently, other erroneous lower bounds have been claimed in [24, (4.1)] for a related problem based on [28, (3.17)].

To correct the situation we first show that with $Z_k := Z_k([-b, -a], [a, b])$ we have

$$\sqrt{Z_k} = E_k([-b, -a]) = E_k([a, b]) = E_k([a/b, 1]),$$

where the last two equalities are immediate from symmetry considerations and scaling. Since any $z_1, \dots, z_k \in \mathbb{C}$ describes a rational function for $E_k([-b, -a])$ in (A.1), the solution to (A.1) describes a rational function that is a candidate for the Zolotarev problem in (1.4) and we have $\sqrt{Z_k} \leq E_k([-b, -a])$. Conversely, taking $R(z)$ as in Theorem 3.3 we get from property (c) that $R(z)$ has a set of poles being closed under complex conjugation. Property (b) tells us that, if p_j is a pole of R , then $-p_j$ is a zero of R . Thus, from Theorem 3.3 we have

$$R(z) = \pm \prod_{j=1}^k \frac{z + \bar{p}_j}{z - p_j},$$

which implies that $E_k([-b, -a]) \leq \max_{z \in [-b, -a]} |R(z)| \leq \sqrt{Z_k}$. Here, in the last inequality we have applied property (a). We conclude that $E_k([-b, -a]) = \sqrt{Z_k}$.

Therefore, an infinite product formula for $E_k([\eta, 1])$ that corrects [27, (1.11)] is obtained by taking square roots (and setting $a/b = \eta$) in Theorem 3.1. That is, for $0 < \eta < 1$ we have

$$(30) \quad E_k([\eta, 1]) = 2\rho^{-k} \prod_{\tau=1}^{\infty} \frac{(1 + \rho^{-8\tau k})^2}{(1 + \rho^{4k} \rho^{-8\tau k})^2}, \quad \rho = \exp\left(\frac{\pi^2}{2\mu(\eta)}\right),$$

where $\mu(\cdot)$ is the Grötzsch ring function. From (A.2), one obtains upper and lower bounds for $E_k([\eta, 1])$ that correct [27, (1.12)], [28, (3.17)], and [32, (15)], namely

$$(31) \quad \frac{2\rho^{-k}}{(1 + \rho^{-4k})^2} \leq E_k([\eta, 1]) \leq \frac{2\rho^{-k}}{1 + \rho^{-4k}} \leq 2\rho^{-k}, \quad \rho = \exp\left(\frac{\pi^2}{2\mu(\eta)}\right).$$

More refined estimates than in (A.3) can be obtained by taking more terms from the infinite product in (A.2).

More recently, the best rational approximation of the sign function on $[-b, -a] \cup [a, b]$ has become important in numerical linear algebra because of a recursive construction of spectral projectors of matrices [24, 30]. In this setting, if $E_{m,n} := E_{m,n}([-b, -a], [a, b])$ then

$$E_{m,n} = \min_{r \in \mathcal{R}_{m,n}} \max_{z \in [-b, -a] \cup [a, b]} |r(z) - \text{sgn}(z)|, \quad \text{sgn}(z) = \begin{cases} 1, & z \in [a, b], \\ -1, & z \in [-b, -a]. \end{cases}$$

Unfortunately, lower and upper bounds for $E_{2k,2k} = E_{2k-1,2k}$ are claimed in [24, (4.1)] based on the erroneous infinite product formula in [28, (3.17)] and for $E_{2k+1,2k+1} = E_{2k+1,2k}$ in [30, (3.8)] by incorrectly citing the fundamental work of Gončar [21, (32)].

We believe it is therefore useful to state infinite product formulas for $E_{k,k}$ and the resulting estimates. We recall from the proof of Theorem 3.1 and Theorem 3.3 that we have

$$E_{k,k} = E_{2\lfloor(k-1)/2\rfloor+1, 2\lfloor k/2\rfloor} = \frac{2\sqrt{Z_k}}{1 + Z_k}, \quad \mu\left(\frac{2\sqrt{Z_k}}{1 + Z_k}\right) = \frac{\mu(Z_k)}{2}.$$

Thus, in the proof of Theorem 3.1 we select $q = \exp(-2\mu(E_{k,k})) = \rho^{-2k}$ and obtain

$$(32) \quad E_{k,k} = 4\rho^{-k} \prod_{\tau=1}^{\infty} \frac{(1 + \rho^{-4\tau k})^4}{(1 + \rho^{2k} \rho^{-4\tau k})^4}, \quad \rho = \exp\left(\frac{\pi^2}{2\mu(a/b)}\right).$$

Again, this infinite product in (A.4) results in asymptotically tight corrected lower and upper bounds on $E_{k,k}$:

$$(33) \quad \frac{4\rho^{-k}}{(1 + \rho^{-2k})^4} \leq E_{k,k} \leq \frac{4\rho^{-k}}{(1 + \rho^{-2k})^2} \leq 4\rho^{-k}, \quad \rho = \exp\left(\frac{\pi^2}{2\mu(a/b)}\right).$$

Similarly, more refined estimates than in (A.5) can be obtained by taking more terms from the infinite product in (A.4).