



Vandermonde matrices with Chebyshev nodes [☆]

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Abstract

For an $N \times N$ Vandermonde matrix $V_N = (\alpha_j^{i-1})_{1 \leq i, j \leq N}$ with translated Chebyshev zero nodes, it is discovered that V_N^T admits an explicit QR decomposition with the R -factor consisting of the coefficients of the translated Chebyshev polynomials. This decomposition then leads to an exact expression for the Frobenius condition number of its submatrix $V_{k,N} = (\alpha_j^{i-1})_{1 \leq i \leq k, 1 \leq j \leq N}$ (so-called a rectangular Vandermonde matrix), bounds on individual singular value, and more. It is explained how these results can be used to establish asymptotically optimal lower bounds on condition numbers of real rectangular Vandermonde matrices and nearly optimally conditioned real rectangular Vandermonde matrices on a given interval. Extensions are also made for V_N with nodes being zeros of any translated orthogonal polynomials other than Chebyshev ones.

Similar results hold for V_N with translated Chebyshev extreme nodes, too, owing to that V_N^T admits an explicit QR-like decomposition.

Close formulas of or tight bounds on the residuals are also presented for the conjugate gradient method, the minimal residual method, and the generalized minimal residual method on certain linear systems $Ax = b$ with A having eigenvalues the same as the nodes mentioned above. As a by-product, they yield positive definite linear systems for which the residuals by the conjugate gradient method are always comparable to the existing error bounds for all iteration steps.

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1. Introduction

Given N numbers $\alpha_1, \alpha_2, \dots, \alpha_N$ called *nodes*, the associated *Vandermonde Matrix* is defined as

$$V_N \stackrel{\text{def}}{=} \begin{pmatrix} 1 & 1 & \dots & 1 \\ \alpha_1 & \alpha_2 & \dots & \alpha_N \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_1^{N-1} & \alpha_2^{N-1} & \dots & \alpha_N^{N-1} \end{pmatrix}. \tag{1.1}$$

V_N appears naturally in polynomial interpolations [6]. For $1 \leq k \leq N$, let

$$V_{k,N} = (\alpha_j^{i-1})_{1 \leq i \leq k, 1 \leq j \leq N}, \quad \text{the first } k \text{ rows of } V_N,$$

so-called a *rectangular Vandermonde matrix*. $V_{k,N}$ appears naturally in the best polynomial fitting in the least squares sense, and, as we shall see later, plays an important role in analyzing the convergence of certain Krylov subspace methods such as the Conjugate Gradient method (CG) for positive definite linear systems, the Minimal Residual method (MINRES) for indefinite Hermitian linear systems, the Generalized Minimal Residual method (GMRES) for normal linear systems. For polynomial fitting applications, the condition number¹ of $V_{k,N}$ may account for the accuracy of the computed best fitting polynomials in the worst case scenario; while for analyzing the convergence of Krylov subspace methods, certain minimizations involving $V_{k,N}$ need to be answered.

In [21], various asymptotically optimal lower bounds on condition numbers of real V_N were established. The key idea was to use the coefficients of Chebyshev polynomials of the first kind to arrive at lower bounds on the norms of V_N^{-1} and explicitly compute the ℓ_∞ -operator norm of V_N^{-1} with translated Chebyshev zero nodes with the help of Gautschi’s formula [12]. Two similar bounds were also obtained by Beckermann [3].

CG is widely used to solve a positive definite linear system $Ax = b$ of order N . In [22], we revisited an example of Meinardus [25], which was used to show that the following well-known and frequently referenced error bound (see, e.g., [8,14,27,30]):

$$\frac{\|r_k\|_{A^{-1}}}{\|r_0\|_{A^{-1}}} \equiv \frac{\|A^{-1}b - x_k\|_A}{\|A^{-1}b\|_A} \leq 2[\Delta_\kappa^k + \Delta_\kappa^{-k}]^{-1} \tag{1.2}$$

was sharp, where $r_k = b - Ax_k$ is the k th CG residual for the k th CG approximation x_k , the M -vector norm $\|z\|_M \stackrel{\text{def}}{=} \sqrt{z^* M z}$, $\kappa \equiv \kappa(A) = \|A\|_2 \|A^{-1}\|_2$ is the spectral condition number, generic notation $\|\cdot\|_2$ is for either the spectral norm (the largest singular value) of a matrix or the euclidian length of a vector, and

$$\Delta_t \stackrel{\text{def}}{=} \frac{\sqrt{t} + 1}{|\sqrt{t} - 1|} \quad \text{for } t > 0, \tag{1.3}$$

that will be used frequently later for different t . But Meinardus [25] did it only for $k = N - 1$, the next-to-the-last CG iteration, for which (1.2) is an equality. In [22], we obtained a close expression of the ratio $\|r_k\|_{A^{-1}}/\|r_0\|_{A^{-1}}$ for all $1 \leq k \leq N - 1$ and in particular we showed that this ratio is always within a factor of $1/\sqrt{2}$ of the upper bound by (1.2).

¹ This statement is only partially true, as often special algorithms that take advantage of its structure yield more accurately computed results than otherwise suggested by the condition number [15].

In this paper, we shall exploit the technique, namely, QR or QR-like decompositions of $V_{k,N}$, that was successfully used in [22], to accomplish three tasks. First we shall investigate the conditioning of $V_{k,N}$ with translated Chebyshev nodes defined in Section 2 and nearly optimally conditioned $V_{k,N}$ if its nodes are restricted to an interval $[\alpha, \beta]$. In particular we will show that with translated Chebyshev nodes on $[\alpha, \beta]$,

$$c_1 N^{d_1} \leq \kappa_F(V_{k,N}) / \rho^{k-1} \leq c_2 N^{d_2}, \tag{1.4}$$

where c_1, c_2, d_1, d_2 are constants, the condition number $\kappa_F(V_{k,N})$ is defined later in (1.7), and

$$\rho = \begin{cases} \max \left\{ \beta^{-1} + \sqrt{1 + \beta^{-2}}, \beta + \sqrt{1 + \beta^2} \right\} & \text{for } -\alpha = \beta, \\ \max \left\{ \left(\sqrt{\beta^{-1}} + \sqrt{1 + \beta^{-1}} \right)^2, \left(1 + \sqrt{1 + \beta} \right)^2 \right\} & \text{for } 0 = \alpha < \beta. \end{cases} \tag{1.5}$$

Our success in [22] relied on solving exactly a minimization problem involving $V_{k,N}$ with translated Chebyshev extreme nodes. As our second task in this paper, we shall solve a few similar minimization problems, each of which relates to residuals of CG, MINRES, and GMRES on certain linear systems and possibly gives extreme examples that are difficult for the methods. The arguments that lead to the solutions to these minimization problems are along the lines in [22] which only dealt with one particular case. This idea of creating extreme examples, especially for CG, works in principle for the symmetric Lanczos algorithm for eigenvalue problems, too, and the interested reader is referred to [20] for how this can be done. Our third task is to establish various inequalities involving the singular values of $V_{k,N}$.

By default, we denote and order the singular values of an n -by- m matrix X as

$$\sigma_1(X) \leq \sigma_2(X) \leq \dots \leq \sigma_{\min\{m,n\}}(X). \tag{1.6}$$

Matrix condition numbers are usually defined for square matrices, but they can be extended without difficulty to non-square matrices. We define X 's Frobenius condition number by

$$\kappa_F(X) \stackrel{\text{def}}{=} \sqrt{\sum_{j=1}^{\min\{m,n\}} [\sigma_j(X)]^2} \sqrt{\sum_{j=1}^{\min\{m,n\}} \frac{1}{[\sigma_j(X)]^2}}. \tag{1.7}$$

The first factor in the right-hand side is just X 's Frobenius norm $\|X\|_F$. If the rank of X is less than $\min\{m, n\}$, then $\sigma_{\min\{m,n\}}(X) = 0$ and thus $\kappa_F(X) = \infty$. Later in Section 3, ℓ_p -condition number $\kappa_p(X)$ will be defined, too, for $1 \leq p \leq \infty$.

The rest of this paper is organized as follows. Section 2 briefly presents relevant preliminary material related to Chebyshev polynomials of the first kind. In Section 3, a lower bound on the ℓ_p -condition number of $V_{k,N}$ with all $\alpha_j \in [\alpha, \beta]$ (a given interval) is established. This bound, combined with later results on $V_{k,N}$ with translated Chebyshev nodes, lead to asymptotically optimal lower bounds in (1.4) and (1.5) for the case $-\alpha = \beta$ and the case $\alpha\beta \geq 0$. Section 4 is devoted to $V_{k,N}$ with translated Chebyshev zero nodes, while Section 5 to $V_{k,N}$ with translated Chebyshev extreme nodes. Possible extensions to $V_{k,N}$ with translated zeros of an orthogonal polynomial are outlined in Section 6. Finally we give some conclusions in Section 7. Some of the proofs for theorems in Sections 4 and 5 are quite long and tedious and thus are postponed to Appendixes A and B.

Notation. Throughout this paper, $\mathbb{C}^{n \times m}$ is the set of all $n \times m$ complex matrices, $\mathbb{C}^n = \mathbb{C}^{n \times 1}$, and $\mathbb{C} = \mathbb{C}^1$. Similarly define $\mathbb{R}^{n \times m}$, \mathbb{R}^n , and \mathbb{R} except replacing the word *complex* by *real*. I_n (or simply I if its dimension is clear from the context) is the $n \times n$ identity matrix, and e_j is its

j th column. $X \preceq Y$ for two Hermitian matrices means that $Y - X$ is positive semidefinite. The superscript “.” takes conjugate transpose while “T” takes transpose only.

We shall also adopt MATLAB-like convention to access the entries of vectors and matrices. $i : j$ is the set of integers from i to j inclusive. For vector u and matrix X , $u_{(j)}$ is u 's j th entry, $X_{(i,j)}$ is X 's (i, j) th entry, $\text{diag}(u)$ is the diagonal matrix with $(\text{diag}(u))_{(j,j)} = u_{(j)}$; X 's submatrices $X_{(k:\ell,i:j)}$, $X_{(k:\ell,:)}$, and $X_{(:,i:j)}$ consist of intersections of row k to row ℓ and column i to column j , row k to row ℓ , and column i to column j , respectively.

$\lfloor \xi \rfloor$ is the largest integer that is no bigger than ξ ; while $\lceil \xi \rceil$ is the smallest integer that is no less than ξ . \sum_j' means the first term is halved, while for \sum_j'' both the first and last terms are halved.

Some of the estimates for condition numbers in this paper are not intended to be best possible but rather to correctly show their asymptotical speeds as k and N go to ∞ . For this purpose, we shall use

$$a_{k,N} \sim b_{k,N} \text{ to mean that there are constants } c_1, c_2, d_1, \text{ and } d_2 \text{ such that } \\ c_1 N^{d_1} \leq a_{k,N}/b_{k,N} \leq c_2 N^{d_2}; \text{ and } a_{k,N} \sim b_{k,N} \text{ if } a_{k,N}/b_{k,N} \rightarrow 1 \text{ as } k, N \rightarrow \infty.$$

2. Chebyshev polynomials

The m th Chebyshev polynomial of the first kind is

$$T_m(t) = \cos(m \arccos t) \quad \text{for } |t| \leq 1, \tag{2.1}$$

$$= \frac{1}{2} \left(t + \sqrt{t^2 - 1} \right)^m + \frac{1}{2} \left(t - \sqrt{t^2 - 1} \right)^m \quad \text{for } |t| \geq 1. \tag{2.2}$$

It frequently shows up in numerical analysis and computations because of its numerous nice properties, for example $|T_m(t)| \leq 1$ for $|t| \leq 1$ and $|T_m(t)|$ grows extremely fast for $|t| > 1$. It can be verified (see, e.g., [22])

$$\left| T_m \left(\frac{1+t}{1-t} \right) \right| = \left| T_m \left(\frac{t+1}{t-1} \right) \right| = \frac{1}{2} [\Delta_t^m + \Delta_t^{-m}] \quad \text{for } 1 \neq t > 0. \tag{2.3}$$

Given two (real or complex) numbers $\omega \neq 0$ and τ , the m th Translated Chebyshev Polynomial in z of degree m is defined by

$$T_m(z; \omega, \tau) \stackrel{\text{def}}{=} T_m(z/\omega + \tau), \tag{2.4}$$

$$= a_{mm}z^m + a_{m-1m}z^{m-1} + \dots + a_{1m}z + a_{0m}, \tag{2.5}$$

where $a_{jm} \equiv a_{jm}(\omega, \tau)$ are functions of ω and τ . Their explicit dependence on ω and τ is often suppressed for convenience. Define

$$\text{Chebyshev zero nodes: } t_{jm} = \cos \theta_{jm}, \quad \theta_{jm} = \frac{2j-1}{2m} \pi, \quad 1 \leq j \leq m, \tag{2.6}$$

$$\text{Chebyshev extreme nodes: } \tau_{jm} = \cos \vartheta_{jm}, \quad \vartheta_{jm} = \frac{j}{m} \pi, \quad 0 \leq j \leq m. \tag{2.7}$$

It can be seen that t_{jm} ($1 \leq j \leq m$) are the zeros of $T_m(t)$, and τ_{jm} ($0 \leq j \leq m$) are the extreme points of $T_m(t)$ in $[-1, 1]$. Define accordingly

Translated Chebyshev zero nodes: $t_{jm}^{tr} = \omega(t_{jm} - \tau), \quad 1 \leq j \leq m, \tag{2.8}$

Translated Chebyshev extreme nodes: $\tau_{jm}^{tr} = \omega(\tau_{jm} - \tau), \quad 0 \leq j \leq m. \tag{2.9}$

Let upper triangular $R_m \in \mathbb{C}^{m \times m}$, a matrix-valued function in ω and τ , be

$$R_m \equiv R_m(\omega, \tau) \stackrel{\text{def}}{=} \begin{pmatrix} a_{00} & a_{01} & a_{02} & \cdots & a_{0m-1} \\ & a_{11} & a_{12} & \cdots & a_{1m-1} \\ & & a_{22} & \cdots & a_{2m-1} \\ & & & \ddots & \vdots \\ & & & & a_{m-1m-1} \end{pmatrix}, \tag{2.10}$$

i.e., the j th column consists of the coefficients of $T_{j-1}(z; \omega, \tau)$. In [21], we defined $S_{m,p}(\omega, \tau)$ as

$$S_{m,p}(\omega, \tau) = \left(\sum_{j=0}^m |a_{jm}|^p \right)^{1/p} \quad \text{for } 1 \leq p \leq \infty.$$

Also explicit formulas were found² for $p = 1$ and $\tau = 0$:

$$S_{m,1}(\omega, 0) = T_m(\iota/\omega) \sim \frac{1}{2} \left(\frac{1}{|\omega|} + \sqrt{1 + \frac{1}{|\omega|^2}} \right)^m, \tag{2.11}$$

where $\iota = \sqrt{-1}$, and for all real τ with $|\tau| \geq 1$:

$$\begin{aligned} S_{m,1}(\omega, \tau) &= T_m(|\tau| + 1/|\omega|) \\ &\sim \frac{1}{2} \left[\left(\frac{1}{|\omega|} + |\tau| \right) + \sqrt{\left(\frac{1}{|\omega|} + |\tau| \right)^2 - 1} \right]^m. \end{aligned} \tag{2.12}$$

In particular for $|\tau| = 1$,

$$S_{m,1}(\omega, 1) \sim \frac{1}{2} \left[\sqrt{\frac{1}{2|\omega|}} + \sqrt{1 + \frac{1}{2|\omega|}} \right]^{2m}. \tag{2.13}$$

No explicit formulas or tight bounds are known for other τ , however. For $p \neq 1$, $S_{m,p}(\omega, \tau)$ relates to $S_{m,1}(\omega, \tau)$ by inequalities

$$(m + 1)^{-1/p'} S_{m,1}(\omega, \tau) \leq S_{m,p}(\omega, \tau) \leq S_{m,1}(\omega, \tau), \tag{2.14}$$

$$\lceil (m + 1)/2 \rceil^{-1/p'} S_{m,1}(\omega, 0) \leq S_{m,p}(\omega, 0) \leq S_{m,1}(\omega, 0), \tag{2.15}$$

where $1/p + 1/p' = 1$ which will be used to define p' throughout the later sections.

In the rest of this paper, by default, $\omega \neq 0$ and τ are two prescribed (real or complex) numbers, but when there is an interval $[\alpha, \beta]$ in the context, they are given by

$$\omega = \frac{\beta - \alpha}{2} > 0, \quad \tau = -\frac{\alpha + \beta}{\beta - \alpha}. \tag{2.16}$$

² Although in [19] these formulas were established with an interval $[\alpha, \beta]$ in the context (see (2.16)), the proofs there can be easily modified for ω and τ that have nothing to do with any interval $[\alpha, \beta]$.

The linear transformation

$$t(z) = \frac{z}{\omega} + \tau = \frac{2}{\beta - \alpha} \left(z - \frac{\alpha + \beta}{2} \right) \tag{2.17}$$

maps $z \in [\alpha, \beta]$ one-to-one and onto $t \in [-1, 1]$.

3. Lower bounds for $\kappa_p(V_{k,N})$

This section concerns V_N with all $\alpha_j \in [\alpha, \beta]$ but otherwise general. The results will be used in the later sections.

We start by defining the ℓ_p vector and operator norm. Given $1 \leq p \leq \infty$, the ℓ_p -norm of n -vector u and the ℓ_p -operator norm of matrix X are defined as

$$\|u\|_p = \left(\sum_{j=1}^n |u_{(j)}|^p \right)^{1/p}, \quad \|X\|_p = \max_{u \neq 0} \frac{\|Xu\|_p}{\|u\|_p}.$$

It can be proved that $\|X\|_p = \|X^T\|_{p'}$; see, e.g., [18]. Define³

$$\text{lub}_p(V_{k,N}) \stackrel{\text{def}}{=} \min_{u \neq 0} \frac{\|V_{k,N}^T u\|_{p'}}{\|u\|_{p'}}, \quad \kappa_p(V_{k,N}) \stackrel{\text{def}}{=} \frac{\|V_{k,N}\|_p}{\text{lub}_p(V_{k,N})}. \tag{3.1}$$

Such definition is unlikely new, and is consistent with the case for $p = 2$ and the square matrix case. In fact $\text{lub}_2(V_{k,N}) = \sigma_1(V_{k,N})$, $V_{k,N}$'s smallest singular value, and for $k = N$, it can be shown that $\text{lub}_p(V_N) = \|V_N^{-1}\|_p^{-1}$.

Theorem 3.1. For $V_{k,N}$ with all nodes $\alpha_j \in [\alpha, \beta]$, we have

$$\text{lub}_p(V_{k,N}) \leq \frac{N^{1/p'}}{S_{k-1,p'}(\omega, \tau)}, \tag{3.2}$$

$$\kappa_p(V_{k,N}) \geq \|V_{k,N}\|_p \frac{S_{k-1,p'}(\omega, \tau)}{N^{1/p'}}, \tag{3.3}$$

where ω and τ are defined as in (2.16).

Proof. Let v be the vector of the coefficients of $T_{k-1}(z; \omega, \tau) \equiv T_{k-1}(z/\omega + \tau)$ such that $v_{(j+1)} = a_{jk-1}$ for $0 \leq j \leq k - 1$. Then

$$V_{k,N}^T v = (T_{k-1}(\alpha_1/\omega + \tau) \quad T_{k-1}(\alpha_2/\omega + \tau) \quad \cdots \quad T_{k-1}(\alpha_N/\omega + \tau))^T,$$

which yields $\|V_{k,N}^T v\|_{p'} \leq N^{1/p'}$ because $|T_{k-1}(z/\omega + \tau)| \leq 1$ for $z \in [\alpha, \beta]$. We therefore have

$$\text{lub}_p(V_{k,N}) = \min_{u \neq 0} \frac{\|V_{k,N}^T u\|_{p'}}{\|u\|_{p'}} \leq \frac{\|V_{k,N}^T v\|_{p'}}{\|v\|_{p'}} \leq \frac{N^{1/p'}}{\left(\sum_{j=0}^{k-1} |a_{j,k-1}|^{p'} \right)^{1/p'}}.$$

This gives (3.2). Eq. (3.3) is the consequence of (3.1) and (3.2). \square

We now specialize Theorem 3.1 to the case $-\alpha = \beta$ or $\alpha\beta \geq 0$.

³ For matrix $X \in \mathbb{C}^{N \times k}$ and $k < N$, it should be defined as $\text{lub}_p(X) = \min_{u \neq 0} \frac{\|Xu\|_p}{\|u\|_p}$.

Theorem 3.2. Let $V_{k,N}$ be with all nodes $\alpha_j \in [\alpha, \beta]$, and suppose $\max_j |\alpha_j| \geq \eta \max\{|\alpha|, |\beta|\}$ for some $1 \geq \eta > 0$.

(1) If $-\alpha = \beta$, then

$$\kappa_p(V_{k,N}) \geq \max\{1, \eta^{k-1} \beta^{k-1}\} \frac{S_{k-1,1}(\beta, 0)}{[k/2]^{1/p} N^{1/p'}} \tag{3.4}$$

$$\sim \frac{1}{2[k/2]^{1/p} N^{1/p'}} \times \max \left\{ \left(\beta^{-1} + \sqrt{1 + \beta^{-2}} \right)^{k-1}, \eta^{k-1} \left(\beta + \sqrt{1 + \beta^2} \right)^{k-1} \right\}. \tag{3.5}$$

(2) If⁴ $0 \leq \alpha < \beta$, then

$$\kappa_p(V_{k,N}) \geq \max\{1, \eta^{k-1} \beta^{k-1}\} \frac{S_{k-1,1}(\omega, \tau)}{k^{1/p} N^{1/p'}} \tag{3.6}$$

$$\geq \max\{1, \eta^{k-1} \beta^{k-1}\} \frac{S_{k-1,1}(\beta/2, 1)}{k^{1/p} N^{1/p'}} \tag{3.7}$$

$$\sim \frac{1}{2k^{1/p} N^{1/p'}} \times \max \left\{ \left(\sqrt{\beta^{-1}} + \sqrt{1 + \beta^{-1}} \right)^{2(k-1)}, \eta^{k-1} \left(1 + \sqrt{1 + \beta} \right)^{2(k-1)} \right\}. \tag{3.8}$$

Proof. Since $\max_j |\alpha_j| \geq \eta \max\{|\alpha|, |\beta|\}$, we have

$$\begin{aligned} \|V_{k,N}\|_p &\geq \max_j \|V_{k,N}^T e_j\|_{p'} = \max_j \left(\sum_{i=0}^{k-1} |\alpha_j|^{ip'} \right)^{1/p'} \\ &\geq \max\{1, \max_j |\alpha_j|^{k-1}\} \\ &\geq \max\{1, \eta^{k-1} |\alpha|^{k-1}, \eta^{k-1} |\beta|^{k-1}\}. \end{aligned} \tag{3.9}$$

Now if $-\alpha = \beta$, then $\omega = \beta$ and $\tau = 0$, and by (2.11) and (2.15)

$$\begin{aligned} S_{k-1,p'}(\beta, 0) &\geq [k/2]^{-1/p} S_{k-1,1}(\beta, 0) \\ &\sim [k/2]^{-1/p} \frac{1}{2} \left(\frac{1}{\beta} + \sqrt{1 + \frac{1}{\beta^2}} \right)^{k-1}. \end{aligned}$$

This, together with Theorem 3.1 and (3.9), lead to (3.4) and (3.5).

If $0 \leq \alpha < \beta$, then $\omega = (\beta - \alpha)/2 \leq \beta/2$ and $\tau \leq -1$. Since $S_{k-1,p'}(\omega, \tau) = S_{k-1,p'}(|\omega|, |\tau|)$ and it is increasing in $|\tau|$ and decreasing in $|\omega|$ [21], we have by (2.13) and (2.14)

⁴ Any result for this case in the rest of this paper holds for the case $\alpha < \beta \leq 0$ as well.

$$\begin{aligned}
 S_{k-1,p'}(\omega, \tau) &\geq k^{-1/p} S_{k-1,1}(\omega, \tau) \\
 &\geq k^{-1/p} S_{k-1,1}(\beta/2, 1) \\
 &\sim k^{-1/p} \frac{1}{2} \left(\sqrt{\beta^{-1}} + \sqrt{1 + \beta^{-1}} \right)^{2(k-1)}.
 \end{aligned}$$

This, together with Theorem 3.1 and (3.9), lead to (3.6), (3.7), and (3.8). \square

Taking $\eta = 1$ in Theorem 3.2 gives better lower bounds, and it is always possible to do so by picking an appropriate (e.g., the smallest) $[\alpha, \beta]$ that contains all α_j . What makes us to have such a factor η is that it gives us some flexibility in applying the theorem later on. One of such occasions is for V_N with translated Chebyshev zero nodes in the next section.

While (3.6) is for all $\alpha_j \in [\alpha, \beta]$ with $0 \leq \alpha$ and possibly $\alpha \neq 0$, (3.7) is actually for all $\alpha_j \in [0, \beta]$ only, i.e., $\alpha = 0$. Asymptotical expansions (3.5) and (3.8) are quite informative:

- (1) $\kappa_p(V_{k,N})$ as a function of k grows at least exponentially;
- (2) Both expressions are smallest at $\beta \approx 1$ which may indicate that the best $\kappa_p(V_{k,N})$, or equivalently the smallest $\kappa_p(V_{k,N})$, may occur for some $V_{k,N}$ with $\max_j |\alpha_j| \approx 1$. This is indeed true; see Theorem 4.4 below.

4. V_N with Chebyshev zero nodes

In this section, V_N has the translated Chebyshev zero nodes $\alpha_j = t_{jN}^{\text{tr}}$ ($1 \leq j \leq N$), except possibly in Theorem 4.4. Set

$$\mathbf{T}_N \stackrel{\text{def}}{=} \begin{pmatrix} T_0(t_{1N}) & T_0(t_{2N}) & \cdots & T_0(t_{NN}) \\ T_1(t_{1N}) & T_1(t_{2N}) & \cdots & T_1(t_{NN}) \\ \vdots & \vdots & & \vdots \\ T_{N-1}(t_{1N}) & T_{N-1}(t_{2N}) & \cdots & T_{N-1}(t_{NN}) \end{pmatrix}. \tag{4.1}$$

Then

$$V_N^T R_N = \mathbf{T}_N^T \tag{4.2}$$

and it can be verified that [10, pp. 34–35]

$$\mathbf{T}_N \mathbf{T}_N^T = (N/2) \Pi^{-1}, \quad \Pi = \text{diag}(2^{-1}, 1, 1, \dots). \tag{4.3}$$

Here $\Pi \in \mathbb{R}^{N \times N}$. In what follows, we shall let Π have a generic dimension determined by the context. Notice that \mathbf{T}_N is real while V_N and R_N may be complex if ω or τ is. Eqs. (4.2) and (4.3) essentially give a QR decomposition for V_N^T after normalizing \mathbf{T}_N^T 's columns to have unit norm. Extracting the first k columns from both sides of $V_N^T = \mathbf{T}_N^T R_N^{-1}$ yields the following theorem.

Theorem 4.1 [20]. *Let V_N have the translated Chebyshev zero nodes $\alpha_j = t_{jN}^{\text{tr}}$ ($1 \leq j \leq N$) defined by (2.6) and (2.8) with arbitrary $\omega \neq 0$ and τ , and let upper triangular R_k be defined as in (2.10) and \mathbf{T}_N as in (4.1). Then $V_{k,N}^T = \mathbf{T}_{k,N}^T R_k^{-1}$, where $\mathbf{T}_{k,N} \stackrel{\text{def}}{=} (\mathbf{T}_N)_{(1:k,:)}$ is \mathbf{T}_N 's first k rows.*

4.1. Condition number $\kappa_F(V_{k,N})$

Let $\bar{V}_{k,N}$ be its complex conjugate. By Theorem 4.1, we have⁵

$$\begin{aligned} \bar{V}_{k,N} V_{k,N}^T &= R_k^{-*} T_{k,N} T_{k,N}^T R_k^{-1} \\ &= R_k^{-*} (T_N T_N^T)_{(1:k, 1:k)} R_k^{-1} \\ &= (N/2) R_k^{-*} \Pi^{-1} R_k^{-1}, \end{aligned} \tag{4.4}$$

$$(\bar{V}_{k,N} V_{k,N}^T)^{-1} = (2/N) R_k \Pi R_k^*. \tag{4.5}$$

Consequently,

$$\begin{aligned} \sum_j [\sigma_j(V_{k,N})]^2 &= \frac{N}{2} \text{trace} \left(R_k^{-*} \Pi^{-1} R_k^{-1} \right) \\ &= \frac{N}{2} \left\| \Pi^{1/2} R_k^{-1} \right\|_F^2, \end{aligned} \tag{4.6}$$

$$\begin{aligned} \text{m} \sum_j \frac{1}{[\sigma_j(V_{k,N})]^2} &= \frac{2}{N} \left\| \Pi^{-1/2} R_k^* \right\|_F^2 \\ &= \frac{2}{N} \sum_{j=0}^{k-1} [S_{j,2}(\omega, \tau)]^2. \end{aligned} \tag{4.7}$$

Eq. (4.6) involves R_k^{-1} , making it a little hard to use without inverting R_k first. We might be better off by using $\sqrt{\sum_j [\sigma_j(V_{k,N})]^2} = \|V_{k,N}\|_F$ when it comes to estimate $\|V_{k,N}\|_F$. Nevertheless it relates the singular values to the coefficients of $T_j(z; \omega, \tau)$ in a nontrivial way.

Theorem 4.2. *Let $V_{k,N}$ have the translated Chebyshev zero nodes defined by (2.6) and (2.8) with arbitrary $\omega \neq 0$ and τ . Then*

$$\kappa_F(V_{k,N}) = \|V_{k,N}\|_F \sqrt{\frac{2}{N} \sum_{j=0}^{k-1} [S_{j,2}(\omega, \tau)]^2}.$$

While this theorem does not require any interval in the context, previously similar estimates (bounds) for the condition numbers of $V_{k,N}$ were done for $\alpha_j = t_{jN}^{\text{tr}}$ on $[\alpha, \beta]$ only with either $-\alpha = \beta$ or $\alpha\beta \geq 0$, $k = N$, and $\kappa_p(V_N)$ for $p = \infty$ in Gautschi [12] and for all $1 \leq p \leq \infty$ in Li [21]. We shall now estimate $\kappa_F(V_{k,N})$ for all $1 \leq k \leq N$.

⁵ One can also have

$$V_{k,N} V_{k,N}^T = (N/2) R_k^{-T} \Pi^{-1} R_k^{-1}, \quad (V_{k,N} V_{k,N}^T)^{-1} = (2/N) R_k \Pi R_k^T.$$

Although they are very similar to (4.4) and (4.5) but can be quite different because ω and/or τ and thus $V_{k,N}$ may possibly be complex. Whether these two identities have any use remains to be seen.

Lemma 4.1. Let $\alpha_j = t_{jN}^{\text{tr}} (1 \leq j \leq N)$ on $[\alpha, \beta]$. Then $\max_j |\alpha_j| = \eta \max\{|\alpha|, |\beta|\}$, where

$$\eta = \begin{cases} \left(\frac{1+\delta}{2} + \frac{1-\delta}{2} \cos \frac{\pi}{2N} \right) \sim 1 - \frac{1-\delta}{16N^2} \pi^2 + \mathcal{O}(N^{-4}), & \text{if } \alpha\beta \geq 0, \\ \left(\frac{1-\delta}{2} + \frac{1+\delta}{2} \cos \frac{\pi}{2N} \right) \sim 1 - \frac{1+\delta}{16N^2} \pi^2 + \mathcal{O}(N^{-4}), & \text{if } \alpha\beta < 0, \end{cases}$$

and $\delta = \min\{|\alpha|, |\beta|\} / \max\{|\alpha|, |\beta|\} \leq 1$. Consequently for $1 \leq k \leq N$

$$\eta^{k-1} \sim \begin{cases} 1 - \frac{(k-1)(1-\delta)}{16N^2} \pi^2 + \mathcal{O}((k-1)^2 N^{-4}), & \text{if } \alpha\beta \geq 0, \\ 1 - \frac{(k-1)(1+\delta)}{16N^2} \pi^2 + \mathcal{O}((k-1)^2 N^{-4}), & \text{if } \alpha\beta < 0. \end{cases}$$

Proof. The expression for η is the consequence of

$$t_{jN}^{\text{tr}} = \omega(t_{jN} - \tau) = \frac{\beta - \alpha}{2} \cos \frac{2j-1}{2N} \pi + \frac{\beta + \alpha}{2}.$$

The asymptotical expansion for η^{k-1} can be gotten through expanding $\exp((k-1) \ln \eta)$. \square

With this lemma, we have

$$\begin{aligned} \|V_{k,N}\|_F &\leq \sqrt{kN} \max\{1, \max_j |t_{jN}^{\text{tr}}|^{k-1}\} \\ &\sim \sqrt{kN} [\max\{1, |\alpha|, |\beta|\}]^{k-1}, \end{aligned} \tag{4.8}$$

$$\begin{aligned} \|V_{k,N}\|_F &\geq \max\{1, \max_j |t_{jN}^{\text{tr}}|^{k-1}\} \\ &\sim [\max\{1, |\alpha|, |\beta|\}]^{k-1}. \end{aligned} \tag{4.9}$$

Together they imply

$$\sqrt{\sum_j [\sigma_j(V_{k,N})]^2} = \|V_{k,N}\|_F \stackrel{N}{\sim} [\max\{1, |\alpha|, |\beta|\}]^{k-1}. \tag{4.10}$$

By (2.14), (4.10), and Theorem 4.2, we have

$$\kappa_F(V_{k,N}) \stackrel{N}{\sim} [\max\{1, |\alpha|, |\beta|\}]^{k-1} \sum_{j=0}^{k-1} S_{j,1}(\omega, \tau). \tag{4.11}$$

Theorem 4.3. Let $V_{k,N}$ have the translated Chebyshev zero nodes on $[\alpha, \beta]$.

(1) If $-\alpha = \beta$, then

$$\kappa_F(V_{k,N}) \stackrel{N}{\sim} \max\{1, \beta^{k-1}\} S_{k-1,1}(\beta, 0) \tag{4.12}$$

$$\stackrel{N}{\sim} \max \left\{ \left(\frac{1}{\beta} + \sqrt{1 + \frac{1}{\beta^2}} \right)^{k-1}, \left(\beta + \sqrt{1 + \beta^2} \right)^{k-1} \right\}. \tag{4.13}$$

Thus those $V_{k,N}$ with $-\alpha = \beta \approx 1$ are nearly optimally conditioned among all $V_{k,N}$ with the translated Chebyshev zero nodes on $[-\beta, \beta]$.

(2) If $0 \leq \alpha < \beta$, then

$$\begin{aligned} \kappa_F(V_{k,N}) &\stackrel{N}{\sim} \max\{1, \beta^{k-1}\} S_{k-1,1}(\omega, \tau) \\ &\geq \max\{1, \beta^{k-1}\} S_{k-1,1}(\beta/2, 1). \end{aligned} \tag{4.14}$$

In particular, if $0 = \alpha < \beta$,

$$\begin{aligned} \kappa_F(V_{k,N}) &\stackrel{N}{\sim} \max \max \{1, \beta^{k-1}\} S_{k-1,1}(\beta/2, 1) \\ &\stackrel{N}{\sim} \max \left\{ \left(\sqrt{\beta^{-1}} + \sqrt{1 + \beta^{-1}} \right)^{2(k-1)}, \left(1 + \sqrt{1 + \beta} \right)^{2(k-1)} \right\}. \end{aligned} \tag{4.15}$$

Thus those $V_{k,N}$ with $\beta \approx 1$ are nearly optimally conditioned among all $V_{k,N}$ with the translated Chebyshev zero nodes on $[0, \beta]$.

Proof. For the case $-\alpha = \beta, \omega = \beta$ and $\tau = 0$, and thus we have (4.12) and (4.13) by (4.11) and (2.11). For the case $\alpha\beta \geq 0$, use (4.11) and (2.12) to complete the proof. \square

Since $\kappa_F(V_N) \stackrel{N}{\sim} \kappa_p(V_N)$, all (4.12)–(4.15) for $k = N$ can be deduced from results in [21]. They, in fact, together with Theorems 3.1 and 3.2 for $k = N$ were the foundation in [21]. Now we have similar conclusions for all $V_{k,N}$ with arbitrary nodes in $[\alpha, \beta]$ for all k . They are summarized in the following theorem, with the help of Theorem 3.2.

Theorem 4.4. *If $-\alpha = \beta$ or $\alpha\beta \geq 0$, then subject to all $\alpha_j \in [\alpha, \beta]$ and $(\max_j |\alpha_j|)^{N-1} \stackrel{N}{\sim} [\max\{|\alpha|, |\beta|\}]^{N-1}$,*

$$\min \kappa_F(V_{k,N}) \stackrel{N}{\sim} [\max\{1, |\alpha|, |\beta|\}]^{k-1} S_{k-1,1}(\omega, \tau),$$

and thus $V_{k,N}$ with $\alpha_j = t_{jN}^{\text{tr}} (1 \leq j \leq N)$ in $[\alpha, \beta]$ is nearly optimally conditioned among all $V_{k,N}$ with nodes in $[\alpha, \beta]$. In particular, subject to the same constraints above,

$$\min \kappa_F(V_{k,N}) \stackrel{N}{\sim} \begin{cases} \text{RHS of (4.13)}, & \text{for } -\alpha = \beta, \\ \text{RHS of (4.15)}, & \text{for } 0 = \alpha < \beta. \end{cases}$$

Furthermore

$$\min_{\alpha_j \in \mathbb{R}} \kappa_F(V_{k,N}) \stackrel{N}{\sim} (1 + \sqrt{2})^{k-1}, \quad \min_{\alpha_j \geq 0} \kappa_F(V_{k,N}) \stackrel{N}{\sim} (1 + \sqrt{2})^{2(k-1)}.$$

But questions such as what asymptotically optimal lower bounds and/or nearly optimally conditioned Vandermonde matrices are for interval with $-\alpha \neq \beta, \alpha < 0$, and $\beta > 0$ were not answered in [19,21]. With Theorem 4.2 here, we are one step closer as we shall explain. Answers to both questions would be firm if we could show that the right-hand sides of (3.3) and (4.11) were equivalent in the sense of $\stackrel{N}{\sim}$. We suspect this would be very much true because it would be reasonable to expect $S_{j,1}(\omega, \tau)$ to be (almost) nondecreasing as j increases, but we have no proof for it for now. So we formulate a conjecture as follows, which has been known to be true for $-\alpha = \beta$ or $\alpha\beta \geq 0$, by examining (2.11) and (2.12).

Conjecture 4.1. *For $\alpha < \beta, \omega$ and τ defined as in (2.16),*

$$\sum_{j=0}^{k-1} S_{j,1}(\omega, \tau) \stackrel{N}{\sim} S_{k-1,1}(\omega, \tau).$$

4.2. Extreme examples for CG, MINRES, and GMRES

A key component in [20,22] for devising examples to achieve the sharpness of the existing error bound (1.2) for CG is the computation of the minimization problem $\min_{|u_{(1)}|=1} \|\text{diag}(g)V_{k,N}^T u\|_2$ for $V_{k,N}$ with the translated Chebyshev zero or extreme nodes on an interval. The convergence analysis of GMRES for $Ax = b$ with normal A ends up with the same computation, too, except possibly with complex α_j .

In this subsection we will present close formulas or tight bounds for similar minimization problems. Extreme examples can then be devised based on them, upon noticing (4.17) and (4.19) below.

Any normal matrix $A \in \mathbb{C}^{N \times N}$ admits the following eigen-decomposition:

$$A = Q\Lambda Q^*, \quad Q^*Q = I_N, \quad \Lambda = \text{diag}(\alpha_1, \alpha_2, \dots, \alpha_N). \tag{4.16}$$

For CG, all $\alpha_j > 0$, and the k th residual r_k satisfies

$$\begin{aligned} \|r_k\|_{A^{-1}} &= \min_{y \in \mathcal{K}_k} \|b - Ay\|_{A^{-1}} \quad [8, \text{p. 306}] \\ &= \min_{|u_{(1)}|=1} \|\text{diag}(g)V_{k+1,N}^T u\|_2, \quad [22] \end{aligned} \tag{4.17}$$

where $\mathcal{K}_k \equiv \mathcal{K}_k(A, b)$ is the k th Krylov subspace of A on b defined as

$$\mathcal{K}_k \equiv \mathcal{K}_k(A, b) \stackrel{\text{def}}{=} \text{span}\{b, Ab, \dots, A^{k-1}b\}, \tag{4.18}$$

$g = A^{-1/2}Q^*b$ and $u \in \mathbb{C}^{k+1}$. In general for GMRES with normal A , including MINRES proposed in [26] for possibly indefinite Hermitian A , the k th residual r_k satisfies

$$\begin{aligned} \|r_k\|_2 &= \min_{y \in \mathcal{K}_k} \|b - Ay\|_2 \quad [26, 28] \\ &= \min_{|u_{(1)}|=1} \|\text{diag}(g)V_{k+1,N}^T u\|_2, \quad [16, 20, 24] \end{aligned} \tag{4.19}$$

where $g = Q^*b$. After substituting k for $k + 1$, the convergence analysis in both (4.18) and (4.20) rests on computing or estimating

$$\min_{|u_{(1)}|=1} \frac{\|\text{diag}(g)V_{k,N}^T u\|_2}{\|g\|_2} = \frac{[e_1^T (\bar{V}_{k,N} [\text{diag}(|g|)]^2 V_{k,N}^T)^{-1} e_1]^{-1/2}}{\|g\|_2}, \tag{4.20}$$

where $|g|$ is the vector obtained by taking entrywise absolute values. In obtaining the equality in (4.20) by Lemma 4.2 below, we have assumed that $\text{diag}(g)V_{k,N}^T$ has rank k .

In light of the CG connection in (4.18), we shall set

$$\kappa \stackrel{\text{def}}{=} \frac{\max_j \alpha_j}{\min_j \alpha_j} = \frac{t_{1N}^{\text{tr}}}{t_{N1}^{\text{tr}}} < \varkappa \stackrel{\text{def}}{=} \frac{\beta}{\alpha}, \tag{4.21}$$

whenever all $\alpha_j = t_{jN}^{\text{tr}}$ on $[\alpha, \beta]$ with $0 \leq \alpha$, for which $|T_j(\tau)| = \frac{1}{2}[\Delta_{\varkappa}^j + \Delta_{\varkappa}^{-j}]$ by (2.3). For some of the quantities in the theorems below that are undefined for $\alpha = 0$, they should be interpreted as by setting $\alpha \rightarrow 0^+$. For example, $\varkappa = +\infty$ and $\Delta_{\varkappa} = 1$ when $\alpha = 0$. In what follows we shall compute the quantity in (4.20) under the following three different situations:

(1) $\alpha_j = t_{jN}^{\text{tr}}$ with $\omega \neq 0$ and τ arbitrary, and $|g_{(j)}| = 1$ ($1 \leq j \leq N$) for which $\|g\|_2 = \sqrt{N}$;

(2) $\alpha_j = t_{jN}^{\text{tr}}$ on $[\alpha, \beta]$ with $0 \leq \alpha$, and $|g_{(j)}| = 1/\sqrt{t_{jN}^{\text{tr}}}$ ($1 \leq j \leq N$) for which

$$\|g\|_2 = \begin{cases} \left[\frac{N}{\sqrt{\alpha\beta}} \cdot \frac{\Delta_{\varkappa}^N - \Delta_{\varkappa}^{-N}}{\Delta_{\varkappa}^N + \Delta_{\varkappa}^{-N}} \right]^{1/2} & \text{for } 0 < \alpha, \\ N\sqrt{2/\beta} & \text{for } 0 = \alpha; \end{cases} \tag{4.22}$$

(3) $\alpha_j = t_{jN}^{\text{tr}}$ on $[\alpha, \beta]$ with $0 \leq \alpha$, and $|g_{(j)}| = \sqrt{t_{jN}^{\text{tr}}}$ ($1 \leq j \leq N$) for which $\|g\|_2 = \sqrt{N(\alpha + \beta)}/2$.

Norm formulas for $\|g\|_2$ in Items 2 and 3 above will be implied in the proofs later. Define

$$\Phi_{\tau,k} = \sum_{j=0}^{k-1} |T_j(\tau)|^2. \tag{4.23}$$

In its present general form, the next lemma was proved in [20]. It was also implied by the proof of [16, Theorem 2.1]. See also [23].

Lemma 4.2. *If Z has full column rank, then*

$$\min_{|u_{(1)}|=1} \|Zu\|_2 = [e_1^T (Z^*Z)^{-1} e_1]^{-1/2}. \tag{4.24}$$

Theorem 4.5. *Let $V_{k,N}$ have the translated Chebyshev zero nodes defined by (2.6) and (2.8) with arbitrary $\omega \neq 0$ and τ , all $|g_{(j)}| = 1$, and let $\Phi_{\tau,k}$ be as in (4.23). Then for $1 \leq k \leq N$*

$$\min_{|u_{(1)}|=1} \frac{\|\text{diag}(g)V_{k,N}^T u\|_2}{\|g\|_2} = (2\Phi_{\tau,k})^{-1/2}. \tag{4.25}$$

If $\alpha_j = t_{jN}^{\text{tr}}$ on $[\alpha, \beta]$ with $0 \leq \alpha$, then for $1 \leq k \leq N$

$$\begin{aligned} (2\Phi_{\tau,k})^{-1/2} &= \min_{|u_{(1)}|=1} \frac{\|\text{diag}(g)V_{k,N}^T u\|_2}{\|g\|_2} \leq 2 \left[\Delta_{\kappa}^{k-1} + \Delta_{\kappa}^{-(k-1)} \right]^{-1} \\ &< 2 \left[\Delta_{\varkappa}^{k-1} + \Delta_{\varkappa}^{-(k-1)} \right]^{-1}. \end{aligned} \tag{4.26}$$

In particular if $\alpha = 0$, then $(2\Phi_{\tau,k})^{-1/2} = 1/\sqrt{2k-1}$.

Proof. In (4.20), $[\text{diag}(|g|^2)]^2 = I_N$. Eq. (4.5) gives

$$e_1^T (\bar{V}_{k,N} V_{k,N}^T)^{-1} e_1 = \frac{1}{N} |a_{00}|^2 + \frac{2}{N} \sum_{j=1}^{k-1} |a_{0j}|^2, \tag{4.27}$$

where $a_{0j} \equiv a_{0j}(\omega, \tau)$ as in (2.5) is the constant term of $T_j(z/\omega + \tau)$, and thus $|a_{0j}| = |T_j(\tau)|$. This gives (4.25). For $[\alpha, \beta]$ with $0 \leq \alpha$, (1.2) implies the “ \leq ” in (4.26). If $\alpha = 0$, then $\tau = -1$ and thus all $|a_{0j}| = 1$. \square

Let us see how tight the existing error bound $2[\Delta_{\kappa}^{k-1} + \Delta_{\kappa}^{-(k-1)}]^{-1}$ is for the case in (4.26) and $0 < \alpha$. Since $\kappa/\varkappa \rightarrow 1$ as $N \rightarrow \infty$, we shall instead use a slightly larger bound $2[\Delta_{\varkappa}^{k-1} + \Delta_{\varkappa}^{-(k-1)}]^{-1}$ in our comparison. We have

$$\frac{\text{RHS of (4.26)}}{\text{LHS of (4.26)}} \leq \sqrt{2} \frac{\left[3(k-1) + 1 + \frac{\Delta_{\varkappa}^{2k-1}}{\Delta_{\varkappa}^2 - 1} \right]^{1/2}}{\Delta_{\varkappa}^{k-1}}$$

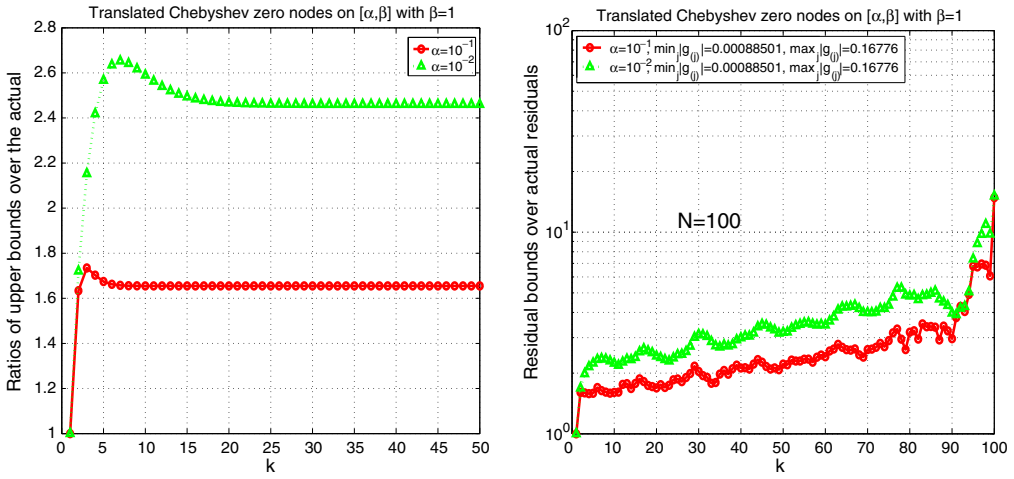


Fig. 4.1. Ratios of $2(\Delta_{\varkappa}^{k-1} + \Delta_{\varkappa}^{-(k-1)})^{-1}$ over $\min_{|u_{(1)}|=1} \|\text{diag}(g)V_{k,N}^T u\|_2 / \|g\|_2$ for $V_{k,N}$ with translated Chebyshev zero nodes on $[\alpha, 1]$ (thus $\varkappa = 1/\alpha$); Left: all $|g_{(j)}| = 1$; Right: random g with $\|g\|_2 = 1$.

$$\begin{aligned} &\leq \sqrt{2} \left[\frac{3(k-1) + 1}{\Delta_{\varkappa}^{2(k-1)}} + \frac{\Delta_{\varkappa}^2}{\Delta_{\varkappa}^2 - 1} \right]^{1/2}, \\ \frac{\text{RHS of (4.26)}}{\text{LHS of (4.26)}} &\rightarrow \frac{\sqrt{2}\Delta_{\varkappa}}{\sqrt{\Delta_{\varkappa}^2 - 1}} = \frac{1 + \sqrt{\varkappa}}{\sqrt{2}\sqrt[4]{\varkappa}} \text{ as } k \rightarrow \infty. \end{aligned}$$

At the left of Fig. 4.1, this ratio is plotted for $1 \leq k \leq 50$ for $\varkappa = 10^1$ and 10^2 , respectively. Notice the ratio quickly converges to

$$\frac{1 + \sqrt{\varkappa}}{\sqrt{2}\sqrt[4]{\varkappa}} = \begin{cases} 1.655068794066460 \dots, & \text{for } \varkappa = 10^1, \\ 2.459674775249768 \dots, & \text{for } \varkappa = 10^2. \end{cases} \tag{4.28}$$

Also plotted at the right of Fig. 4.1 are the ratios

$$\frac{2[\Delta_{\varkappa}^{k-1} + \Delta_{\varkappa}^{-(k-1)}]^{-1}}{\min_{|u_{(1)}|=1} \|\text{diag}(\tilde{g})V_{k,N}^T u\|_2 / \|\tilde{g}\|_2},$$

where \tilde{g} is a random vector. It shows that the existing upper bound is still pretty good for the case, too. This can be partially explained. Let g be as in Theorem 4.5, $\tilde{g} \in \mathbb{C}^N$, and

$$\gamma_{\min} = \frac{\sqrt{N} \min_j |\tilde{g}_{(j)}|}{\|\tilde{g}\|_2}, \quad \gamma_{\max} = \frac{\sqrt{N} \max_j |\tilde{g}_{(j)}|}{\|\tilde{g}\|_2}.$$

Then

$$\gamma_{\min} \frac{\|\text{diag}(g)V_{k,N}^T u\|_2}{\|g\|_2} \leq \min_{|u_{(1)}|=1} \frac{\|\text{diag}(\tilde{g})V_{k,N}^T u\|_2}{\|\tilde{g}\|_2} \leq \gamma_{\max} \frac{\|\text{diag}(g)V_{k,N}^T u\|_2}{\|g\|_2}. \tag{4.29}$$

Since $\min_{|u_{(1)}|=1} \frac{\|\text{diag}(g)V_{k,N}^T u\|_2}{\|g\|_2}$ is comparable to $2[\Delta_{\varkappa}^{k-1} + \Delta_{\varkappa}^{-(k-1)}]^{-1}$, the quantity in the middle of (4.29) should be, too, unless possibly when the magnitude of $|\tilde{g}_{(j)}|$ varies too much.

Proofs of the next two theorems are rather complicated and technical and thus will be postponed to Appendix A.

Theorem 4.6. Let $\alpha_j = t_{jN}^{\text{tr}}$ on $[\alpha, \beta]$ with $0 \leq \alpha$, and $|g_{(j)}| = 1/\sqrt{t_{jN}^{\text{tr}}}$ ($1 \leq j \leq N$). If $0 < \alpha$, then we have for $1 \leq k \leq N$

$$\min_{|u_{(1)}|=1} \frac{\|\text{diag}(g)V_{k,N}^T u\|_2}{\|g\|_2} = \varrho_{k-1} \times 2 \left[\Delta_{\alpha}^{k-1} + \Delta_{\alpha}^{-(k-1)} \right]^{-1}, \tag{4.30}$$

where ϱ_{k-1} , strictly decreasing in k , is given by

$$\frac{1}{2} \left(1 - \frac{\Delta_{\alpha}^{2(N-1)} - \Delta_{\alpha}^2}{\Delta_{\alpha}^{2N} - 1} \right) \leq \varrho_{k-1}^2 = \frac{1}{2} \left(1 - \frac{\Delta_{\alpha}^{2(k-1)} - \Delta_{\alpha}^{2[N-(k-1)]}}{\Delta_{\alpha}^{2N} - 1} \right) \leq 1.$$

If $\alpha = 0$, then we have for $1 \leq k \leq N$

$$\min_{|u_{(1)}|=1} \frac{\|\text{diag}(g)V_{k,N}^T u\|_2}{\|g\|_2} = \left[1 - \frac{k-1}{N} \right]^{1/2}. \tag{4.31}$$

Theorem 4.7. Let $\alpha_j = t_{jN}^{\text{tr}}$ on $[\alpha, \beta]$ with $0 \leq \alpha$, and $|g_{(j)}| = \sqrt{t_{jN}^{\text{tr}}}$ ($1 \leq j \leq N$). If $0 < \alpha$, then we have for $1 \leq k \leq N$

$$\sqrt{\frac{1}{\alpha+1}} \sqrt{\frac{1}{2\Phi_{\tau,k}+1}} \leq \min_{|u_{(1)}|=1} \frac{\|\text{diag}(g)V_{k,N}^T u\|_2}{\|g\|_2} \leq \sqrt{\frac{2\alpha}{\alpha+1}} \sqrt{\frac{1}{2\Phi_{\tau,k}+1}}, \tag{4.32}$$

where $\Phi_{\tau,k}$ is as in (4.23). If $\alpha = 0$, then we have for $1 \leq k \leq N$

$$\min_{|u_{(1)}|=1} \frac{\|\text{diag}(g)V_{k,N}^T u\|_2}{\|g\|_2} = \sqrt{\frac{3}{k(4k^2-1)}}. \tag{4.33}$$

4.3. Bounds on individual singular values

Let the diagonal entries of the right-hand side of (4.5) be d_j ($1 \leq j \leq k$). Then

$$d_1 = \frac{2}{N} \sum_{i=0}^{k-1} |a_{0i}|^2, \quad d_j = \frac{2}{N} \sum_{i=j-1}^{k-1} |a_{j-i}|^2 \quad \text{for } 2 \leq j \leq k. \tag{4.34}$$

By Schur’s theorem [5, p. 35], we have

Theorem 4.8. Let $V_{k,N}$ have the translated Chebyshev zero nodes defined by (2.6) and (2.8) with arbitrary $\omega \neq 0$ and τ . The set of eigenvalues of $(\bar{V}_{k,N} V_{k,N}^T)^{-1}$ which is $\{[\sigma_j(V_{k,N})]^{-2}\}_{j=1}^k$ majorizes $\{d_j\}_{j=1}^k$ defined as in (4.34).

Recall our default ordering (1.6) on singular values to get

$$[\sigma_1(V_{k,N})]^{-2} \geq [\sigma_2(V_{k,N})]^{-2} \geq \dots \geq [\sigma_k(V_{k,N})]^{-2}.$$

What the majorization in Theorem 4.8 means is if we let $\{d_j^\downarrow\}_{j=1}^k$ be the non-increasing reordering of $\{d_j\}_{j=1}^k$, i.e.,

$$d_1^\downarrow \geq d_2^\downarrow \geq \dots \geq d_k^\downarrow,$$

then

$$\sum_{j=1}^i [\sigma_j(V_{k,N})]^{-2} \geq \sum_{j=1}^i d_j^\downarrow \quad \text{for } 1 \leq i \leq k, \tag{4.35}$$

which can also be equivalently stated as

$$\sum_{j=i}^k [\sigma_j(V_{k,N})]^{-2} \leq \sum_{j=i}^k d_j^\downarrow \quad \text{for } 1 \leq i \leq k. \tag{4.36}$$

Corollary 4.1. *Under the conditions of Theorem 4.8,*

$$\sigma_i(V_{k,N}) \geq \left[\sum_{j=i}^k d_j^\downarrow \right]^{-1/2} \quad \text{for } 1 \leq i \leq k, \tag{4.37}$$

$$[d_1^\downarrow]^{-1/2} \geq \sigma_1(V_{k,N}) \geq \left[\sum_{j=1}^k d_j^\downarrow \right]^{-1/2}. \tag{4.38}$$

Proof. Eq. (4.36) implies

$$[\sigma_i(V_{k,N})]^{-2} \leq \sum_{j=i}^k d_j^\downarrow \quad \text{for } 1 \leq i \leq k,$$

which yields (4.37). Take $i = 1$ in (4.35), combining with (4.37) for $i = 1$, to get (4.38). \square

The lower bounds in (4.37) are guaranteed very sharp for $i = 1$ because of (4.38), but may not be so for $i \neq 1$. Our numerical calculations for various interval $[\alpha, \beta]$ show that they are pretty good for the first few smallest singular values, and then deteriorate as i becomes bigger. But for $\max\{|\alpha|, |\beta|\} \approx 1$, the lower bounds are sharp for both ends of singular values (i.e., the largest and smallest ones).

Exactly the same thing can be done with (4.4) upon extracting the diagonal entries of $R_k^{-*} \Pi^{-1} R_k^{-1}$. But these diagonal entries relate to the coefficients in a much more complicated way. We shall not pursue this here.

5. V_N with Chebyshev extreme nodes

For the sake of presentation, throughout this section,

$$n = N - 1,$$

and V_N will have nodes $\alpha_{j+1} = \tau_{jn}^{\text{tr}}$ for $0 \leq j \leq n$ as defined in (2.7). Set

$$S_N \stackrel{\text{def}}{=} \begin{pmatrix} T_0(\tau_{0n}) & T_0(\tau_{1n}) & \dots & T_0(\tau_{nn}) \\ T_1(\tau_{0n}) & T_1(\tau_{1n}) & \dots & T_1(\tau_{nn}) \\ \vdots & \vdots & \dots & \vdots \\ T_N(\tau_{0n}) & T_N(\tau_{1n}) & \dots & T_N(\tau_{nn}) \end{pmatrix}. \tag{5.1}$$

Then $V_N^T R_N = S_N^T$. S_N is always real, while V_N and R_N may not. Let

$$\Omega = \text{diag}(2^{-1}, 1, 1, \dots, 1, 2^{-1}) \in \mathbb{R}^{N \times N}, \tag{5.2}$$

and define

$$\mathcal{Y} \stackrel{\text{def}}{=} S_N \Omega S_N^T = \frac{n}{2} \Omega^{-1}. \tag{5.3}$$

The last equality is well-known; see [2, p. 33]. Now $V_N^T = S_N^T R_N^{-1}$. Extracting the first k columns from both sides yields the following theorem.

Theorem 5.1 [22]. *Let V_N have the translated Chebyshev extreme nodes $\alpha_{j+1} = \tau_{jn}^{\text{tr}}$ ($0 \leq j \leq n$) defined by (2.7) and (2.9) with arbitrary $\omega \neq 0$ and τ , and let upper triangular R_k be defined as in (2.10) and S_N as in (5.1). Then $V_{k,N}^T = S_{k,N}^T R_k^{-1}$, where $S_{k,N} = (S_N)_{(1:k,:)}$ is S_N 's first k rows.*

5.1. Condition number $\kappa_F(V_{k,N})$

A rough bound for $\mathcal{Y} = (n/2)\Omega^{-1}$ is

$$\frac{n}{2} I_N \leq \mathcal{Y} \leq n I_N, \tag{5.4}$$

which is probably good enough for most occasions. Eq. (5.4) implies immediately

$$\frac{n}{2} I_k \leq \mathcal{Y}_{(1:k,1:k)} \leq n I_k, \quad \frac{1}{n} I_k \leq [\mathcal{Y}_{(1:k,1:k)}]^{-1} \leq \frac{2}{n} I_k. \tag{5.5}$$

By Theorem 5.1, similarly to the derivations in (4.4) and (4.5), we have⁶

$$\begin{aligned} \bar{V}_{k,N} \Omega V_{k,N}^T &= R_k^{-*} S_{k,N} \Omega S_{k,N}^T R_k^{-1} \\ &= R_k^{-*} (S_N \Omega S_N^T)_{(1:k,1:k)} R_k^{-1} \\ &= R_k^{-*} \mathcal{Y}_{(1:k,1:k)} R_k^{-1}, \end{aligned} \tag{5.6}$$

$$\left(\bar{V}_{k,N} \Omega V_{k,N}^T \right)^{-1} = R_k [\mathcal{Y}_{(1:k,1:k)}]^{-1} R_k^*. \tag{5.7}$$

Since $(1/2)I_N \leq \Omega \leq I_N$ and (5.5), we have

$$\begin{aligned} \frac{1}{2} \bar{V}_{k,N} V_{k,N}^T &\leq \bar{V}_{k,N} \Omega V_{k,N}^T \leq \bar{V}_{k,N} V_{k,N}^T, \\ \frac{n}{2} R_k^{-*} R_k^{-1} &\leq R_k^{-*} \mathcal{Y}_{(1:k,1:k)} R_k^{-1} \leq n R_k^{-*} R_k^{-1}, \\ \left(\bar{V}_{k,N} V_{k,N}^T \right)^{-1} &\leq \left(\bar{V}_{k,N} \Omega V_{k,N}^T \right)^{-1} \leq 2 \left(\bar{V}_{k,N} V_{k,N}^T \right)^{-1}, \\ \frac{1}{n} R_k R_k^* &\leq R_k [\mathcal{Y}_{(1:k,1:k)}]^{-1} R_k^* \leq \frac{2}{n} R_k R_k^*. \end{aligned}$$

⁶ Again one can also have

$$V_{k,N} \Omega V_{k,N}^T = (n/2) R_k^{-T} \mathcal{Y}_{(1:k,1:k)} R_k^{-1}, \quad (V_{k,N} \Omega V_{k,N}^T)^{-1} = (2/n) R_k [\mathcal{Y}_{(1:k,1:k)}]^{-1} R_k^T,$$

similarly to (5.6) and (5.7).

Consequently,

$$\frac{n}{2} \|R_k^{-1}\|_F^2 \leq \sum_j [\sigma_j(V_{k,N})]^2 \leq 2n \|R_k^{-1}\|_F^2, \tag{5.8}$$

$$\frac{1}{2n} \sum_{j=0}^{k-1} [S_{j,2}(\omega, \tau)]^2 \leq \sum_j \frac{1}{[\sigma_j(V_{k,N})]^2} \leq \frac{2}{n} \sum_{j=0}^{k-1} [S_{j,2}(\omega, \tau)]^2. \tag{5.9}$$

Theorem 5.2. *Let $V_{k,N}$ have the translated Chebyshev extreme nodes τ_{jn}^{tr} defined by (2.7) and (2.9) with arbitrary $\omega \neq 0$ and τ . Then*

$$\|V_{k,N}\|_F \sqrt{\frac{1}{2n} \sum_{j=0}^{k-1} [S_{j,2}(\omega, \tau)]^2} \leq \kappa_F(V_{k,N}) \leq \|V_{k,N}\|_F \sqrt{\frac{2}{n} \sum_{j=0}^{k-1} [S_{j,2}(\omega, \tau)]^2}.$$

As what we did for Theorem 4.2, we may specialize this theorem onto interval $[\alpha, \beta]$ with $-\alpha = \beta$ or $\alpha\beta \geq 0$ in almost the same way to conclude that Theorems 4.3 and 4.4 remain true with all occurrences of the translated Chebyshev zero nodes replaced by the translated Chebyshev extreme nodes. Detail is omitted.

5.2. *Extreme examples for CG, MINRES, and GMRES*

V_N here provides another example to achieve the sharpness of the existing error bound for CG, as well as many examples with closed formulas for or tight bounds on MINRES and GMRES residuals. We shall compute or estimate

$$\min_{|u_{(1)}|=1} \frac{\|\text{diag}(g)V_{k,N}^T u\|_2}{\|g\|_2} = \frac{[e_1^T (\bar{V}_{k,N} [\text{diag}(|g|)]^2 V_{k,N}^T)^{-1} e_1]^{-1/2}}{\|g\|_2} \tag{5.10}$$

under the following three different situations. In obtaining the equality in (5.10) by Lemma 4.2, we have assumed that $\text{diag}(g)V_{k,N}^T$ has rank k . Similarly to (4.21), we also define κ and \varkappa , but now the two are equal:

$$\kappa \stackrel{\text{def}}{=} \frac{\max_j \tau_{jn}^{\text{tr}}}{\min_j \tau_{jn}^{\text{tr}}} = \frac{\tau_{0n}^{\text{tr}}}{\tau_{nn}^{\text{tr}}} \equiv \varkappa \stackrel{\text{def}}{=} \frac{\beta}{\alpha}, \tag{5.11}$$

whenever $\alpha_{j+1} = \tau_{jn}^{\text{tr}}$ on $[\alpha, \beta]$ with $0 \leq \alpha$, for which $|T_j(\tau)| = \frac{1}{2}(\Delta_\kappa^j + \Delta_\kappa^{-j})$.

- (1) $\alpha_{j+1} = \tau_{jn}^{\text{tr}}$ with $\omega \neq 0$ and τ arbitrary, and for $1 \leq j \leq N$

$$|g_{(j)}| = \sqrt{\Omega_{(j,j)}} \tag{5.12}$$

for which $\|g\|_2 = \sqrt{n}$;

(2) $\alpha_{j+1} = \tau_{jn}^{\text{tr}}$ on $[\alpha, \beta]$ with $0 < \alpha$, and

$$|g_{(j+1)}| = \begin{cases} \sqrt{1/\tau_{jn}^{\text{tr}}}, & \text{for } j \in \{0, n\}, \\ \sqrt{2/\tau_{jn}^{\text{tr}}}, & \text{for } 1 \leq j \leq n - 1 \end{cases} \tag{5.13}$$

for which [22]

$$\|g\|_2 = \left[\frac{2n}{\omega\sqrt{\tau^2 - 1}} \cdot \frac{\Delta_k^n + \Delta_k^{-n}}{\Delta_k^n - \Delta_k^{-n}} \right]^{1/2};$$

(3) $\alpha_{j+1} = \tau_{jn}^{\text{tr}}$ on $[\alpha, \beta]$ with $0 \leq \alpha$, and

$$|g_{(j+1)}| = \begin{cases} \sqrt{\tau_{jn}^{\text{tr}}}, & \text{for } j \in \{0, n\}, \\ \sqrt{2\tau_{jn}^{\text{tr}}}, & \text{for } 1 \leq j \leq n - 1 \end{cases} \tag{5.14}$$

for which $\|g\|_2 = \sqrt{n(\alpha + \beta)}$.

Note the case for (5.13) has already been dealt with in [22]. Define

$$\Psi_{\tau,k} = \begin{cases} \sum_{j=0}^{k-1} |T_j(\tau)|^2, & \text{for } 1 \leq k \leq n, \\ \sum_{j=0}^{k-1} |T_j(\tau)|^2, & \text{for } k = N. \end{cases} \tag{5.15}$$

Theorem 5.3. Let $V_{k,N}$ have the translated Chebyshev extreme nodes defined by (2.7) and (2.9) with arbitrary $\omega \neq 0$ and τ , and let g be as in (5.12). Then for $1 \leq k \leq N$

$$\min_{|u_{(1)}|=1} \frac{\|\text{diag}(g)V_{k,N}^T u\|_2}{\sqrt{n}} = (2\Psi_{\tau,k})^{-1/2}. \tag{5.16}$$

If $\alpha_{j+1} = \tau_{jn}^{\text{tr}}$ on $[\alpha, \beta]$ with $0 < \alpha$, then for $1 \leq k \leq N$

$$(2\Psi_{\tau,k})^{-1/2} = \min_{|u_{(1)}|=1} \frac{\|\text{diag}(g)V_{k,N}^T u\|_2}{\sqrt{n}} \leq 2[\Delta_k^{k-1} + \Delta_k^{-(k-1)}]^{-1}. \tag{5.17}$$

In particular if $\alpha = 0$, then $(2\Psi_{\tau,k})^{-1/2} = 1/\sqrt{2k - 1}$ for $1 \leq k \leq n$ and $1/\sqrt{2n}$ for $k = N$.

Proof. Note $[\text{diag}(|g|)]^2 = \Omega$. By (5.7) and (5.10), we have

$$\begin{aligned} \min_{|u_{(1)}|=1} \|\text{diag}(g)V_{k,N}^T u\|_2 &= [e_1^T (\bar{V}_{k,N} \Omega V_{k,N}^T)^{-1} e_1]^{-1/2} \\ &= [y^* [\mathcal{T}_{(1:k,1:k)}]^{-1} y]^{-1/2}, \end{aligned}$$

where $y \in \mathbb{C}^k$ and $y_{(j+1)} = a_{0j} = T_j(\tau)$. This gives (5.16). Eq. (5.17) follows from (5.16) and the existing CG error bound (1.2). If $\alpha = 0$, then $\tau = -1$ and thus all $|a_{0j}| = 1$. \square

Li [22] obtained the following theorem in which (5.18) for $k = N$ is due to [25].

Theorem 5.4 [22]. Let $0 < \alpha < \beta$, $g \in \mathbb{R}^N$ as in (5.13), and $V_{k,N}$ have the translated Chebyshev extreme nodes. Then for $1 \leq k \leq N$

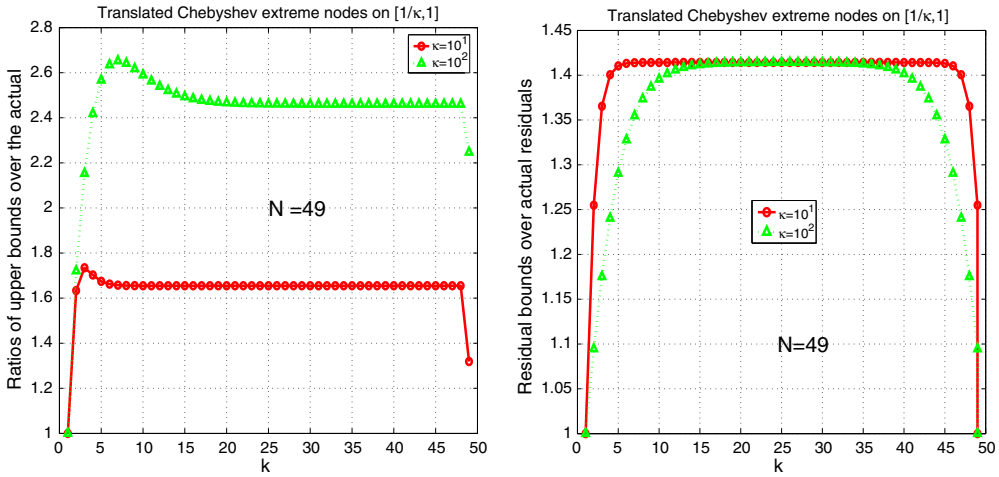


Fig. 5.1. Ratios of $2[\Delta_\kappa^{k-1} + \Delta_\kappa^{-(k-1)}]^{-1}$ over $\min_{|u_{(1)}|=1} \frac{\|\text{diag}(g)V_{k,N}^T u\|_2}{\|g\|_2}$, where $\alpha_{j+1} = \tau_{j_n}^{\text{tr}}$ on $[1/\kappa, 1]$. Left: g as in (5.12); Right: g as in (5.13).

$$\min_{|u_{(1)}|=1} \frac{\|\text{diag}(g)V_{k,N}^T u\|_2}{\|g\|_2} = \rho_{k-1} \times 2 \left[\Delta_\kappa^{k-1} + \Delta_\kappa^{-(k-1)} \right]^{-1}, \tag{5.18}$$

where

$$\frac{1}{2} < \frac{1}{2} \left(1 + \frac{2\Delta_\kappa^n}{\Delta_\kappa^{2n} + 1} \right) \leq \rho_{k-1}^2 = \frac{1}{2} \left(1 + \frac{\Delta_\kappa^{2(k-1)} + \Delta_\kappa^{2[n-(k-1)]}}{\Delta_\kappa^{2n} + 1} \right) \leq 1. \tag{5.19}$$

Fig. 5.1 plots the ratio of $2[\Delta_\kappa^{k-1} + \Delta_\kappa^{-(k-1)}]^{-1}$ over (5.10) for $\alpha_{j+1} = \tau_{j_n}^{\text{tr}}$ on $[1/\kappa, 1]$ with two different g . It is interesting to notice a sudden drop at $k = N$ for g as in (5.12), and for g as in (5.13), the ratio is one at $k = 1$ and N and for all other k the ratios is no bigger than $\sqrt{2}$, as guaranteed by Theorem 5.4. Proof of the next theorem is given in Appendix B.

Theorem 5.5. Let $0 \leq \alpha < \beta$, $g \in \mathbb{R}^N$ as in (5.14), and $V_{k,N}$ have the translated Chebyshev extreme nodes. If $0 < \alpha$, we have for $1 \leq k \leq N$

$$\sqrt{\frac{1}{\kappa + 1}} \Xi^{-1/2} \leq \min_{|u_{(1)}|=1} \frac{\|\text{diag}(g)V_{k,N}^T u\|_2}{\|g\|_2} \leq \sqrt{\frac{2\kappa}{\kappa + 1}} \Xi^{-1/2}, \tag{5.20}$$

where $\Xi = 2\Psi_{\tau,k} + 1 + \eta$, $\Psi_{\tau,k}$ is as in (5.15) and $\eta = 0$ for $k \leq n$ and $\eta = |T_N(\tau)|^2$ for $k = N$. In particular, if $\alpha = 0$, then we have

$$\min_{|u_{(1)}|=1} \frac{\|\text{diag}(g)V_{k,N}^T u\|_2}{\|g\|_2} = \sqrt{\frac{3}{k(4k^2 - 1)}} \quad \text{for } 1 \leq k \leq n, \tag{5.21}$$

and it is zero for $k = N$.

5.3. Bounds on individual singular values

Let the diagonal entries of $R_k[\Upsilon_{(1:k,1:k)}]^{-1}R_k^*$ be

$$\delta_j = e_j^T R_k[\Upsilon_{(1:k,1:k)}]^{-1} R_k^* e_j \quad \text{for } 1 \leq j \leq k. \tag{5.22}$$

By Schur’s theorem [5, p. 35], we have

Theorem 5.6. *Let $V_{k,N}$ have the translated Chebyshev extreme nodes defined by (2.7) and (2.9) with arbitrary $\omega \neq 0$ and τ . The set of eigenvalues of $(\bar{V}_{k,N}\Omega V_{k,N}^T)^{-1}$ which is $\{[\sigma_j(V_{k,N}\Omega^{1/2})]^{-2}\}_{j=1}^k$ majorizes $\{\delta_j\}_{j=1}^k$ defined as in (5.22).*

Let the nonincreasing re-ordering of δ_j ’s be δ_j^\downarrow ’s, i.e.,

$$\delta_1^\downarrow \geq \delta_2^\downarrow \geq \dots \geq \delta_k^\downarrow.$$

Theorem 5.6 implies, upon noticing $\frac{1}{\sqrt{2}}\sigma_j(V_{k,N}) \leq \sigma_j(V_{k,N}\Omega^{1/2}) \leq \sigma_j(V_{k,N})$

$$\sum_{j=1}^i [\sigma_j(V_{k,N})]^{-2} \geq \frac{1}{2} \sum_{j=1}^i \delta_j^\downarrow \quad \text{for } 1 \leq i \leq k, \tag{5.23}$$

$$\sum_{j=i}^k [\sigma_j(V_{k,N})]^{-2} \leq \sum_{j=i}^k \delta_j^\downarrow \quad \text{for } 1 \leq i \leq k. \tag{5.24}$$

Corollary 5.1. *Under the conditions of Theorem 5.6,*

$$\sigma_i(V_{k,N}) \geq \left[\sum_{j=i}^k \delta_j^\downarrow \right]^{-1/2} \quad \text{for } 1 \leq i \leq k, \tag{5.25}$$

$$\sqrt{2} \left[\delta_1^\downarrow \right]^{-1/2} \geq \sigma_1(V_{k,N}) \geq \left[\sum_{j=1}^k \delta_j^\downarrow \right]^{-1/2}. \tag{5.26}$$

Proof. Eq. (5.24) implies

$$[\sigma_i(V_{k,N})]^{-2} \leq \sum_{j=i}^k \delta_j^\downarrow \quad \text{for } 1 \leq i \leq k,$$

which yields (5.25). Take $i = 1$ in (5.23), combining with (5.25) for $i = 1$, to get (5.26). \square

Our comments at the end of Section 4.3 apply here, too.

6. V_N with other orthogonal polynomial zero nodes

Part of the material in Section 4 can be naturally extended to V_N whose nodes are the zeros of the n th translated orthogonal polynomial from any orthogonal polynomial system. We shall only provide an outline here. Let $p_j(t)$, $j = 0, 1, 2, \dots$, denote a sequence of *normalized* orthogonal polynomials with respect to some weight function $w(t)$ on an interval which may be open, half

open, or closed. For a list of well-known orthogonal polynomials such as T_m , Legendre polynomials, etc., the reader is referred to [7, p. 57] or any books on orthogonal polynomials. Orthogonal polynomials have many beautiful properties. Useful to us here is that $p_m(t)$ is guaranteed to have exactly m distinct zeros⁷ t_{jm} , $j = 1, 2, \dots, m$, in the interval, and [13]

$$\sum_{j=1}^m \lambda_{jm} p_r(t_{jm}) p_s(t_{jm}) = \begin{cases} 1, & \text{if } r = s, \\ 0, & \text{otherwise,} \end{cases} \quad \text{for } 0 \leq r, s \leq m - 1 \tag{6.1}$$

as the result of the fact that the Gaussian quadrature formula

$$\int \phi(t) w(t) dt \approx \sum_{j=1}^m \omega_{jm} \phi(t_{jm})$$

is exact for all polynomials of degree no higher than $2m - 1$ and

$$\int p_r(t) p_s(t) w(t) dt = 0 \quad \text{for } r \neq s \text{ and } 1 \text{ for } r = s,$$

where the integral is taken over the support of $w(t)$, ω_{jm} are Christoffel numbers for p_m . For numerical values of the nodes and Christoffel numbers for various orthogonal polynomials, the reader is referred to [1].

Given $\omega \neq 0$ and τ , define translated orthogonal polynomials by

$$p_m(z; \omega, \tau) \stackrel{\text{def}}{=} p_m(z/\omega + \tau), \\ = a_{mm} z^m + a_{m-1m} z^{m-1} + \dots + a_{1m} z + a_{0m},$$

whose zeros are

$$t_{jm}^{\text{tr}} = \omega(t_{jm} - \tau), \quad 1 \leq j \leq m.$$

Let V_N be with $\alpha_j = t_{jN}^{\text{tr}}$ and set R_N as in (2.10) but with a_{ij} here. Define

$$\mathbf{P}_N \stackrel{\text{def}}{=} \begin{pmatrix} p_0(t_{1N}) & p_0(t_{2N}) & \cdots & p_0(t_{NN}) \\ p_1(t_{1N}) & p_1(t_{2N}) & \cdots & p_1(t_{NN}) \\ \vdots & \vdots & & \vdots \\ p_{N-1}(t_{1N}) & p_{N-1}(t_{2N}) & \cdots & p_{N-1}(t_{NN}) \end{pmatrix}. \tag{6.2}$$

Then $V_N^T R_N = \mathbf{P}_N^T$, and

$$\mathbf{P}_N \Omega_N \mathbf{P}_N^T = I_N, \tag{6.3}$$

where $\Omega_N = \text{diag}(\omega_{1N}, \omega_{2N}, \dots, \omega_{NN})$. Therefore $V_N^T = \mathbf{P}_N^T R_N^{-1}$. Extracting the first k columns from both sides yields $V_{k,N}^T = \mathbf{P}_{k,N}^T R_k^{-1}$, similarly to Theorem 4.1, where $\mathbf{P}_{k,N} = (\mathbf{P}_N)_{(1:k,:)}$ is \mathbf{P}_N 's first k rows.

⁷ Up to now, t_{jm} is reserved for the zeros of the m th Chebyshev polynomial of the first kind. It, along with other previously reserved notation, will be reassigned in this section.

Let $\Omega_{k,N} = (\Omega_N)_{(1:k,1:k)}$. We have

$$\begin{aligned} \bar{V}_{k,N} \Omega_{k,N} V_{k,N}^T &= R_k^{-*} P_{k,N} \Omega_{k,N} P_{k,N}^T R_k^{-1} \\ &= R_k^{-*} (P_N \Omega_N P_N^T)_{(1:k,1:k)} R_k^{-1} \\ &= R_k^{-*} R_k^{-1}, \end{aligned} \tag{6.4}$$

$$(\bar{V}_{k,N} \Omega_{k,N} V_{k,N}^T)^{-1} = R_k R_k^*. \tag{6.5}$$

Upon noticing $(\min_j \omega_{jN}) I_k \leq \Omega_{k,N} \leq (\max_j \omega_{jN}) I_k$, we have

$$\frac{1}{\max_j \omega_{jN}} \|R_k^{-1}\|_F^2 \leq \sum_j [\sigma_j(V_{k,N})]^2 \leq \frac{1}{\min_j \omega_{jN}} \|R_k^{-1}\|_F^2, \tag{6.6}$$

$$(\min_j \omega_{jN}) \|R_k\|_F^2 \leq \sum_j \frac{1}{[\sigma_j(V_{k,N})]^2} \leq (\max_j \omega_{jN}) \|R_k\|_F^2. \tag{6.7}$$

Now bounds on $\kappa_F(V_{k,N})$ can be easily obtained in terms of a_{ij} . For CG, MINRES, or GMRES residuals, we have exactly

$$\min_{|u_{(1)}|=1} \|\text{diag}(g) V_{k,N}^T u\|_2 = \left[\sum_{j=0}^{k-1} |p_j(\tau)|^2 \right]^{-1/2}, \tag{6.8}$$

where $g \in \mathbb{C}^N$ with $|g_{(j)}| = \sqrt{\omega_{jN}}$. We may also get bounds on individual singular value $\sigma_j(V_{k,N})$, following the lines of previous sections. For the similarity reason, detail is omitted.

7. Conclusions

Vandermonde matrices with translated Chebyshev zero and extreme nodes are shown to have various interesting properties, derived from simple QR or QR-like decompositions. These decompositions allow us to obtain the behavior of their condition numbers, and bounds on their singular values.

This simple QR-like decomposition for V_N with translated Chebyshev zero nodes is shared by a much larger class of V_N , i.e., those with nodes being translated zeros of any orthogonal polynomial. Consequently we can get about the same things as what we can get for V_N with translated Chebyshev zero nodes.

There are two immediate applications of studying Vandermonde matrices with translated Chebyshev nodes. The first one is to establish asymptotically optimal lower bounds on condition numbers of real *rectangular* Vandermonde matrices and to establish nearly optimally conditioned real *rectangular* Vandermonde matrices on a given interval. Previously similar results were obtained for real *square* Vandermonde matrices in [3,19,21], except in [19,21] where rectangular Vandermonde matrices were discussed but the results there were not satisfactory. The second application is their implications to the convergence analysis of CG, MINRES, and GMRES. It is observed that superlinear convergence [4,29] often occurs for CG; while the existing error bound [17,25] only guarantees linear convergence. Results in this paper can be used to construct examples as in [20,22] for which errors of approximations by CG are comparable to the existing error bounds at all iteration steps.

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Appendix A. Proofs of Theorems 4.6 and 4.7

Lemma A.1. Let $\theta_{kN} = \frac{2k-1}{2N}\pi$ ($1 \leq k \leq N$), and ℓ an integer. Then

$$\sum_{k=1}^N \cos \ell \theta_{kN} = \begin{cases} (-1)^m N, & \text{if } \ell = 2mN \text{ for some integer } m, \\ 0, & \text{otherwise.} \end{cases} \tag{A.1}$$

Proof. This is most likely well-known and can be verified by calculations. See also [20]. \square

Lemma A.2. Let $\Gamma = \text{diag}(\mu + \nu \cos \theta_{1N}, \dots, \mu + \nu \cos \theta_{NN})$, \mathbf{T}_N as in (4.1), Π as in (4.3), and define $\Theta_{\mu,\nu} = \mathbf{T}_N \Gamma \mathbf{T}_N^T$. Then

$$\Theta_{\mu,\nu} = \frac{N}{4}(2\mu\Pi^{-1} + \nu\Pi^{-1}H\Pi^{-1}) = \frac{N}{4}\Pi^{-1}(2\mu\Pi + \nu H)\Pi^{-1},$$

where $H \in \mathbb{R}^{N \times N}$ is tridiagonal with diagonal entries 0 and off-diagonal entries 1.

Proof. For $0 \leq i, j \leq N - 1$,

$$\begin{aligned} (\mathbf{T}_N \Gamma \mathbf{T}_N^T)_{(i+1,j+1)} &= \sum_{k=1}^N (\mathbf{T}_N)_{(i+1,k)}(\mu + \nu \cos \theta_{kN})(\mathbf{T}_N^T)_{(k,j+1)} \\ &= \sum_{k=1}^N T_i(t_{kN})(\mu + \nu \cos \theta_{kN})T_j(t_{kN}) \\ &= \sum_{k=1}^N \cos i\theta_{kN}(\mu + \nu \cos \theta_{kN}) \cos j\theta_{kN} \\ &= \mu \sum_{k=1}^N \cos i\theta_{kN} \cos j\theta_{kN} + \nu \sum_{k=1}^N \cos i\theta_{kN} \cos \theta_{kN} \cos j\theta_{kN}. \end{aligned} \tag{A.2}$$

So $\Theta_{\mu,\nu} = \mu\Theta_{1,0} + \nu\Theta_{0,1}$, where

$$\begin{aligned} (\Theta_{1,0})_{(i+1,j+1)} &= \sum_{k=1}^N \cos i\theta_{kN} \cos j\theta_{kN}, \\ (\Theta_{0,1})_{(i+1,j+1)} &= \sum_{k=1}^N \cos i\theta_{kN} \cos \theta_{kN} \cos j\theta_{kN}. \end{aligned}$$

It is known $\Theta_{1,0} = \frac{N}{2}\Pi^{-1}$ already in (4.3). It remains to compute $\Theta_{0,1}$.

$$4 \sum_{k=1}^N \cos i\theta_{kN} \cos \theta_{kN} \cos j\theta_{kN} = \sum_{k=1}^N \cos(i + j + 1)\theta_{kN} + \sum_{k=1}^N \cos(i + j - 1)\theta_{kN} \\ + \sum_{k=1}^N \cos(i - j + 1)\theta_{kN} + \sum_{k=1}^N \cos(i - j - 1)\theta_{kN}.$$

Apply Lemma A.1 to conclude $\Theta_{0,1} = \frac{N}{4} \Pi^{-1} H \Pi^{-1}$ whose verification is straightforward, albeit tedious. \square

Lemma A.3. Let $m \leq N$ and $\xi \in \mathbb{C}$ such that $(-2\xi\Pi + H)_{(1:m,1:m)}$ is nonsingular. Then the first entry of the solution to $(-2\xi\Pi + H)_{(1:m,1:m)}y = e_1$ is

$$y_{(1)} = \begin{cases} \frac{\gamma_-^m - \gamma_+^m}{\sqrt{\xi^2 - 1}(\gamma_-^m + \gamma_+^m)} & \text{for } \xi \notin \{1, -1\}, \\ -m & \text{for } \xi = 1, \\ m & \text{for } \xi = -1, \end{cases}$$

where $\gamma_{\pm} = \xi \pm \sqrt{\xi^2 - 1}$.

Proof. This is essentially [22, Lemma 3.4] when $\xi \notin \{1, -1\}$. It can be verified that $y_{(j)} = \xi^{j-1}(m - j + 1)$ when $\xi = \pm 1$. \square

Proof of Theorem 4.6. We use (4.20). Let

$$\Gamma = \text{diag}(t_{1N}^{\text{tr}}, t_{2N}^{\text{tr}}, \dots, t_{NN}^{\text{tr}}) \equiv \text{diag}(\mu + \nu \cos \theta_{1N}, \dots, \mu + \nu \cos \theta_{NN}),$$

where $\mu = -\omega\tau$ and $\nu = \omega$. Then

$$V_{k,N}[\text{diag}(|g|)]^2 V_{k,N}^T = V_{k,N} \Gamma^{-1} V_{k,N}^T \\ = \begin{pmatrix} e^T \\ V_{k-1,N} \Gamma \end{pmatrix} \Gamma^{-1} \begin{pmatrix} e & \Gamma V_{k-1,N}^T \end{pmatrix} \\ = \begin{pmatrix} e^T \Gamma^{-1} e & e^T V_{k-1,N}^T \Gamma \\ V_{k-1,N} e & V_{k-1,N} \Gamma V_{k-1,N}^T \end{pmatrix},$$

where $e = (1, 1, \dots, 1)^T$. Notice $V_{k-1,N}^T = T_{k-1,N}^T R_{k-1}^{-1}$ by Theorem 4.1 to get

$$V_{k-1,N} e = V_{k-1,N} V_{k-1,N}^T e_1 \\ = R_{k-1}^{-T} (\Theta_{1,0})_{(1:k-1,1:k-1)} R_{k-1}^{-1} e_1 \\ = R_{k-1}^{-T} (\Theta_{1,0})_{(1:k-1,1:k-1)} e_1, \\ V_{k-1,N} \Gamma V_{k-1,N}^T = R_{k-1}^{-T} T_{k-1,N} \Gamma T_{k-1,N}^T R_{k-1}^{-1} \\ = R_{k-1}^{-T} (\Theta_{\mu,\nu})_{(1:k-1,1:k-1)} R_{k-1}^{-1},$$

where $\Theta_{\mu,\nu}$ is as in Lemma A.2. Recall⁸

⁸ This is well-known. See, e.g., [9, pp. 102–103], [31, p. 23].

$$\begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}^{-1} = \begin{pmatrix} C_{11}^{-1} & -C_{11}^{-1}B_{12}B_{22}^{-1} \\ -B_{22}^{-1}B_{21}C_{11}^{-1} & B_{22}^{-1} + B_{22}^{-1}B_{21}C_{11}^{-1}B_{12}B_{22}^{-1} \end{pmatrix},$$

assuming all inversions exist, where $C_{11} = B_{11} - B_{12}B_{22}^{-1}B_{21}$. We have

$$e_1^T(V_{k,N}[\text{diag}(g)]^2V_{k,N}^T)^{-1}e_1 = [\zeta - e^T V_{k-1,N}^T(V_{k-1,N}\Gamma V_{k-1,N}^T)^{-1}V_{k-1,N}e]^{-1}, \tag{A.3}$$

where $\zeta = e^T \Gamma^{-1}e$. But

$$\begin{aligned} & e^T V_{k-1,N}^T(V_{k-1,N}\Gamma V_{k-1,N}^T)^{-1}V_{k-1,N}e \\ &= e_1^T(\Theta_{1,0})_{(1:k-1,1:k-1)}[(\Theta_{\mu,\nu})_{(1:k-1,1:k-1)}]^{-1}(\Theta_{1,0})_{(1:k-1,1:k-1)}e_1 \\ &= N^2 e_1^T[(\Theta_{\mu,\nu})_{(1:k-1,1:k-1)}]^{-1}e_1. \end{aligned} \tag{A.4}$$

Consider now $\alpha > 0$. Then $\tau < -1$. For $k \leq N$, by Lemma A.3,

$$\begin{aligned} e_1^T[(\Theta_{\mu,\nu})_{(1:k-1,1:k-1)}]^{-1}e_1 &= N^{-1}e_1^T[(2\mu\Pi + \nu H)_{(1:k-1,1:k-1)}]^{-1}e_1 \\ &= \frac{1}{N\omega}e_1^T[(-2\tau\Pi + H)_{(1:k-1,1:k-1)}]^{-1}e_1 \\ &= \frac{1}{N\omega} \frac{\gamma_-^{k-1} - \gamma_+^{k-1}}{\sqrt{\tau^2 - 1}(\gamma_-^{k-1} + \gamma_+^{k-1})}, \end{aligned} \tag{A.5}$$

where $\gamma_{\pm} = \tau \pm \sqrt{\tau^2 - 1}$. Since $\zeta = \|g\|_2^2$, we have by (4.20) and (A.3)–(A.5)

$$\min_{|u_{(1)}|=1} \frac{\|\text{diag}(g)V_{k,N}^T u\|_2}{\|g\|_2} = \left[1 - \frac{N}{\omega\zeta\sqrt{\tau^2 - 1}} \frac{\gamma_-^{k-1} - \gamma_+^{k-1}}{\gamma_-^{k-1} + \gamma_+^{k-1}} \right]^{1/2}. \tag{A.6}$$

We now compute $\omega\zeta\sqrt{\tau^2 - 1}$. Let $f(z) = T_N(z/\omega + \tau)$. We have

$$\zeta = \|g\|_2^2 = \sum_{j=1}^N \frac{1}{t_{jN}^{\text{tr}}} = -\frac{f'(0)}{f(0)} = -\frac{T'_N(\tau)}{\omega T_N(\tau)}.$$

Recall (2.2) and [7, p. 37]

$$2T'_N(t) = N \frac{(t + \sqrt{t^2 - 1})^N - (t - \sqrt{t^2 - 1})^N}{\sqrt{t^2 - 1}},$$

to get $2T_N(\tau) = \gamma_+^N + \gamma_-^N$ and $2T'_N(\tau) = N(\gamma_+^N - \gamma_-^N)/\sqrt{\tau^2 - 1}$. Therefore,

$$\omega\zeta\sqrt{\tau^2 - 1} = N \frac{\gamma_-^N - \gamma_+^N}{\gamma_-^N + \gamma_+^N}.$$

Eq. (A.6) now implies

$$\min_{|u_{(1)}|=1} \frac{\|\text{diag}(g)V_{k,N}^T u\|_2}{\|g\|_2} = \left[1 - \frac{\gamma_-^N + \gamma_+^N}{\gamma_-^N - \gamma_+^N} \frac{\gamma_-^{k-1} - \gamma_+^{k-1}}{\gamma_-^{k-1} + \gamma_+^{k-1}} \right]^{1/2}. \tag{A.7}$$

For $\tau = -(\beta + \alpha)/(\beta - \alpha) = -(\varkappa + 1)/(\varkappa - 1)$,

$$\gamma_-^{k-1} = (-1)^{k-1} \Delta_{\varkappa}^{k-1}, \quad \gamma_+^{k-1} = (-1)^{k-1} \Delta_{\varkappa}^{-(k-1)},$$

and therefore

$$\min_{|u_{(1)}|=1} \frac{\|\text{diag}(g)V_{k,N}^T u\|_2}{\|g\|_2} = \left[1 - \frac{\Delta_\zeta^N + \Delta_\zeta^{-N} \Delta_\zeta^{k-1} - \Delta_\zeta^{-(k-1)}}{\Delta_\zeta^N - \Delta_\zeta^{-N} \Delta_\zeta^{k-1} + \Delta_\zeta^{-(k-1)}} \right]^{1/2} \tag{A.8}$$

$$= \varrho_{k-1} \times 2 \left[\Delta_\zeta^{k-1} + \Delta_\zeta^{-(k-1)} \right]^{-1}, \tag{A.9}$$

where

$$\begin{aligned} \varrho_{k-1} &\stackrel{\text{def}}{=} \frac{\text{RHS of (A.8)}}{2[\Delta_\zeta^{k-1} + \Delta_\zeta^{-(k-1)}]^{-1}} \\ &= \left[\frac{(\Delta_\zeta^{k-1} + \Delta_\zeta^{-(k-1)})^2}{4} - \frac{(\Delta_\zeta^N + \Delta_\zeta^{-N})(\Delta_\zeta^{2(k-1)} - \Delta_\zeta^{-2(k-1)})}{4(\Delta_\zeta^N - \Delta_\zeta^{-N})} \right]^{1/2} \\ &= \left[\frac{1}{2} \frac{(\Delta_\zeta^{k-1} + \Delta_\zeta^{-(k-1)})(\Delta_\zeta^{N-(k-1)} - \Delta_\zeta^{-[N-(k-1)]})}{\Delta_\zeta^N - \Delta_\zeta^{-N}} \right]^{1/2} \\ &= \left[\frac{1}{2} \frac{(\Delta_\zeta^{2(k-1)} + 1)(\Delta_\zeta^{2[N-(k-1)]} - 1)}{\Delta_\zeta^{2N} - 1} \right]^{1/2}. \end{aligned}$$

Since $\Delta_\zeta > 1$, we have

$$\frac{1}{2} \left(1 - \frac{\Delta_\zeta^{2(N-1)} - \Delta_\zeta^2}{\Delta_\zeta^{2N} - 1} \right) \leq \varrho_{k-1}^2 = \frac{1}{2} \left(1 - \frac{\Delta_\zeta^{2(k-1)} - \Delta_\zeta^{2[N-(k-1)]}}{\Delta_\zeta^{2N} - 1} \right) \leq 1,$$

as expected. Eq. (4.31) for $\alpha = 0$ can be obtained by examining the proof above upon setting $\tau = -1$ and noticing $T_N(-1) = (-1)^N$, $T'_N(-1) = -(-1)^N N^2$, $\zeta = N^2/\omega$, and $e_1^T [(\Theta_{\mu,v})_{(1:k-1,1:k-1)}]^{-1} e_1 = \frac{k-1}{N\omega}$. \square

Proof of Theorem 4.7. Again we will use (4.20). Let Γ be as in the proof of Theorem 4.6. Then

$$V_{k,N}[\text{diag}(|g|)]^2 V_{k,N}^T = V_{k,N} \Gamma V_{k,N}^T = R_k^{-T} (\Theta_{\mu,v})_{(1:k,1:k)} R_k^{-1},$$

where $\Theta_{\mu,v}$ is as in Lemma A.2. Set $y = R_k^T e_1$. We have

$$\begin{aligned} e_1^T (V_{k,N}[\text{diag}(g)]^2 V_{k,N}^T)^{-1} e_1 &= e_1^T R_k [(\Theta_{\mu,v})_{(1:k,1:k)}]^{-1} R_k^T e_1 \\ &= y^T \left[\frac{N}{4} \Pi^{-1} (2\mu \Pi + \nu H) \Pi^{-1} \right]_{(1:k,1:k)}^{-1} y \\ &= \frac{4}{N\omega} z^T [(-2\tau \Pi + H)_{(1:k,1:k)}]^{-1} z, \end{aligned}$$

where $z = y$ except its first entry $z_{(1)} = y_{(1)}/2$. Note $y_{(j+1)} = T_j(\tau)$, and thus

$$\|z\|_2^2 = \frac{1}{4} + \sum_{j=1}^{k-1} |T_j(\tau)|^2 = \frac{1}{2} + \Phi_{\tau,k}.$$

Since $\|g\|_2^2 = \sum_{j=1}^N \omega(\cos \theta_{jN} - \tau) = -N\omega\tau = N(\alpha + \beta)/2$, we have by (4.20),

$$\left(\min_{|u_{(1)}|=1} \frac{\|\text{diag}(g)V_{k,N}^T u\|_2}{\|g\|_2} \right)^2 = \frac{1}{4} \frac{\beta - \alpha}{\beta + \alpha} [z^T [(-2\tau\Pi + H)_{(1:k,1:k)}]^{-1} z]^{-1}. \tag{A.10}$$

When $\alpha > 0$, $\tau = -(\varkappa + 1)/(\varkappa - 1) < -1$ and⁹

$$\frac{2}{\varkappa - 1} I_N = (|\tau| - 1)I_N \leq -2\tau\Pi + H \leq 2(|\tau| + 1)I_N = \frac{4\varkappa}{\varkappa - 1} I_N,$$

which gives

$$\frac{\varkappa - 1}{4\varkappa} I_N \leq (-2\tau\Pi + H)^{-1} \leq \frac{\varkappa - 1}{2} I_N.$$

Finally

$$\frac{1}{2(\varkappa + 1)} \|z\|_2^{-2} \leq \left(\min_{|u_{(1)}|=1} \frac{\|\text{diag}(g)V_{k,N}^T u\|_2}{\|g\|_2} \right)^2 \leq \frac{\varkappa}{\varkappa + 1} \|z\|_2^{-2},$$

as was to be shown for (4.32). Now if $\alpha = 0$, then $\tau = -1$, $T_j(\tau) = (-1)^j$, $z = (1/2, -1, 1, -1, \dots)^T$, and $(2\Pi + H)_{(1:k,1:k)} = LL^T$, where $L \in \mathbb{R}^{k \times k}$ is lower bi-diagonal with the main diagonal entries 1 and the off-diagonal entries 1. So the right-hand side of (A.10) is

$$\frac{1}{4} \|L^{-1}z\|_2^{-2} = \frac{3}{k(4k^2 - 1)}$$

and (4.33) now follows. \square

Appendix B. Proof of Theorem 5.5

Lemma B.1. Let $\vartheta_{kn} = \pi k/n$ ($0 \leq k \leq n$), and ℓ an integer. Then

$$\sum_{k=0}^n \cos \ell \vartheta_{kn} = \begin{cases} N, & \text{if } \ell = 2mn \text{ for some integer } m, \\ 0, & \text{if } \ell \text{ is odd,} \\ 1, & \text{if } \ell \text{ is even, but } \ell \neq 2mn \text{ for any integer } m. \end{cases} \tag{B.1}$$

Proof. This is most likely well-known and can be verified by calculations. See also [22]. \square

Lemma B.2 [22]. Let $\Gamma = \text{diag}(\mu + \nu \cos \vartheta_{0n}, \mu + \nu \cos \vartheta_{1n}, \dots, \mu + \nu \cos \vartheta_{nn})$ and define $\Upsilon_{\mu,\nu} \stackrel{\text{def}}{=} \mathbf{S}_N \Omega \Gamma \mathbf{S}_N^T$, where $\mu, \nu \in \mathbb{C}$. We have

$$\Upsilon_{\mu,\nu} = \frac{n}{4} \Omega^{-1} (2\mu\Omega + \nu H) \Omega^{-1}, \tag{B.2}$$

where H is the same as the one in Lemma A.2.

⁹ Better bounds can be obtained as follows. We note $-2\tau\Pi + H = -2(\tau + 1)\Pi + (2\Pi + H)$, and thus

$$\left[(|\tau| - 1) + 4 \sin^2 \frac{1}{2(2k + 1)} \pi \right] I_k \leq (-2\tau\Pi + H)_{(1:k,1:k)} \leq \left[2(|\tau| - 1) + 4 \sin^2 \frac{2k - 1}{2(2k + 1)} \pi \right] I_k$$

because $(2\Pi + H)_{(1:k,1:k)}$ is symmetric with eigenvalues [11] $4 \sin^2 \frac{2j-1}{2(2k+1)} \pi$ for $1 \leq j \leq k$. The improvements based upon this are more significantly for small k and become increasingly negligible for big k .

Proof of Theorem 5.5. We use (5.10). Let

$\Gamma = \text{diag}(\tau_{0n}^{\text{tr}}, \tau_{1n}^{\text{tr}}, \dots, \tau_{nn}^{\text{tr}}) \equiv \text{diag}(\mu + \nu \cos \vartheta_{0n}, \mu + \nu \cos \vartheta_{1n}, \dots, \mu + \nu \cos \vartheta_{nn})$, where $\mu = -\omega\tau$ and $\nu = \omega$ as in (2.16). Then

$$\begin{aligned} V_{k,N}[\text{diag}(|g|)]^2 V_{k,N}^T &= 2V_{k,N} \Omega \Gamma V_{k,N}^T \\ &= 2R_k^{-T} S_{k,N} \Omega \Gamma S_{k,N}^T R_k^{-1} \\ &= 2R_k^{-T} (\Upsilon_{\mu,\nu})_{(1:k,1:k)} R_k^{-1}, \\ e_1^T (V_{k,N}[\text{diag}(|g|)]^2 V_{k,N}^T)^{-1} e_1 &= \frac{1}{2} e_1^T R_k [(\Upsilon_{\mu,\nu})_{(1:k,1:k)}]^{-1} R_k^T e_1 \\ &= \frac{1}{2} y^T \left[\frac{n}{4} \Omega^{-1} (2\mu\Omega + \nu H) \Omega^{-1} \right]_{(1:k,1:k)}^{-1} y \\ &= \frac{2}{n\omega} z^T [(-2\tau\Omega + H)_{(1:k,1:k)}]^{-1} z, \end{aligned}$$

where $y = R_k^T e_1$, $z = y$ except its first entry $z_{(1)} = y_{(1)}/2$ for $k \leq n$ and if $k = N$, $z_{(N)} = y_{(N)}/2$, too. Since $y_{(j+1)} = T_j(\tau)$,

$$\|z\|_2^2 = \begin{cases} \frac{1}{4} + \sum_{j=1}^{k-1} |T_j(\tau)|^2, & \text{if } k \leq n, \\ \frac{1}{4} + \sum_{j=1}^{n-1} |T_j(\tau)|^2 + \frac{1}{4} |T_N(\tau)|^2, & \text{if } k = N \end{cases} = \frac{1}{2} + \Psi_{\tau,k} + \frac{1}{2}\eta.$$

Since $\|g\|_2^2 = 2 \sum_{j=0}^n \omega(\cos \vartheta_{jn} - \tau) - (\alpha + \beta) = -2N\omega\tau - (\alpha + \beta) = n(\alpha + \beta)$, we have by (5.10),

$$\left(\min_{|u_{(1)}|=1} \frac{\|\text{diag}(g) V_{k,N}^T u\|_2}{\|g\|_2} \right)^2 = \frac{1}{4} \frac{\beta - \alpha}{\beta + \alpha} [z^T [(-2\tau\Omega + H)_{(1:k,1:k)}]^{-1} z]^{-1}. \tag{B.3}$$

When $\alpha > 0$, $\tau = -(\kappa + 1)/(\kappa - 1) < -1$, and¹⁰

$$\frac{2}{\kappa - 1} I_N = (|\tau| - 1) I_N \leq -2\tau\Omega + H \leq 2(|\tau| + 1) I_N = \frac{4\kappa}{\kappa - 1} I_N,$$

which gives

$$\frac{\kappa - 1}{4\kappa} I_N \leq (-2\tau\Omega + H)^{-1} \leq \frac{\kappa - 1}{2} I_N.$$

Finally

$$\frac{1}{2(\kappa + 1)} \|z\|_2^{-2} \leq \left(\min_{|u_{(1)}|=1} \frac{\|\text{diag}(g) V_{k,N}^T u\|_2}{\|g\|_2} \right)^2 \leq \frac{\kappa}{\kappa + 1} \|z\|_2^{-2},$$

as was to be shown for the case $\alpha > 0$. Now if $\alpha = 0$ and $k \leq n$, the right-hand sides of (A.10) and (B.3) are the same, and thus no additional proof is needed; if $\alpha = 0$ and $k = N$, then the right-hand side of (B.3) is no longer well defined because $2\Omega + H$ is singular, but its left-hand side is and it is equal to zero. To see this, we notice $\tau_{nn}^{\text{tr}} = \alpha = 0$ and all other $\tau_{jn}^{\text{tr}} > 0$. Let $v \in \mathbb{R}^N$ with $v_{(j+1)}(0 \leq j \leq n)$ being the coefficient of t^j in

$$\phi_n(t) = \prod_{j=0}^{n-1} (\tau_{jn}^{\text{tr}} - t) \Big/ \prod_{j=0}^{n-1} \tau_{jn}^{\text{tr}}.$$

¹⁰ As noted previously in the proof of Theorem 4.7, slightly better bounds can be obtained, too.

Obviously $v_{(1)} = \phi(0) = 1$. It can be seen that $\text{diag}(g)V_N^T v = 0$ which implies the left-hand side of (B.3) is zero. \square

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