University of Kentucky Lexington

Department of Mathematics Technical Report 05-02

Vandermonde Matrices with Chebyshev Nodes[1]

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January 2005

ABSTRACT

For $n \times n$ Vandermonde matrix $V_n = (\alpha_j^{i-1})_{1 \le i\, j \le n}$ 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 of degree less than n. This decomposition then leads to an exact expression for the condition number of its submatrix $V_{k,n} = (\alpha_j^{i-1})_{1 \le i \le k, 1 \le j \le n}$ (so-called rectangular Vandermonde matrix), bounds on individual singular value, and more. It is explained that how these results can be used to establish asymptotically optimal lower bounds on condition numbers of real rectangular Vandermonde matrices and nearly optimal 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.

It is also discovered that for V_{n+1} with translated Chebyshev extreme nodes, V_{n+1}^T admits an explicit QR-like decomposition with the same R-factor, but the Q-factor is no longer has orthogonal columns, except Q^TQ taking a special friendly form. This QR-like decomposition also yields similar conclusions to those for V_n with translated Chebyshev zero nodes.

Applications to the study of sharpness in existing error bounds for the conjugate gradient method and the minimal residual method for linear systems and the symmetric Lanczos method for eigenvalue problems are also discussed.

[1]This report is available on the web at `http://www.ms.uky.edu/~math/MAreport/`.

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Vandermonde Matrices with Chebyshev Nodes

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Abstract

For $n \times n$ Vandermonde matrix $V_n = (\alpha_j^{i-1})_{1 \le i\, j \le n}$ 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 of degree less than n. This decomposition then leads to an exact expression for the condition number of its submatrix $V_{k,n} = (\alpha_j^{i-1})_{1 \le i \le k, 1 \le j \le n}$ (so-called rectangular Vandermonde matrix), bounds on individual singular value, and more. It is explained that how these results can be used to establish asymptotically optimal lower bounds on condition numbers of real rectangular Vandermonde matrices and nearly optimal 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.

It is also discovered that for V_{n+1} with translated Chebyshev extreme nodes, V_{n+1}^T admits an explicit QR-like decomposition with the same R-factor, but the Q-factor is no longer has orthogonal columns, except Q^TQ taking a special friendly form. This QR-like decomposition also yields similar conclusions to those for V_n with translated Chebyshev zero nodes.

Applications to the study of sharpness in existing error bounds for the conjugate gradient method and the minimal residual method for linear systems and the symmetric Lanczos method for eigenvalue problems are also discussed.

1 Introduction

Given n numbers $\alpha_1, \alpha_2, \cdots, \alpha_n$ called *nodes*, the associated *Vandermonde Matrix* is defined as

$$V_n \stackrel{\text{def}}{=} \begin{pmatrix} 1 & 1 & \cdots & 1 \\ \alpha_1 & \alpha_2 & \cdots & \alpha_n \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_1^{n-1} & \alpha_2^{n-1} & \cdots & \alpha_n^{n-1} \end{pmatrix}. \tag{1.1}$$

In [10], we established various asymptotically optimal lower bounds on condition numbers of real V_n. 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 the explicit computation of the ℓ_∞-operator norm of V_n^{-1} with (translated) Chebyshev zero nodes with the help of Gautschi's formula [6]. Two similar bounds were also obtained by Beckermann [2].

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This paper is devoted to the study of V_n with (translated) Chebyshev zero and extreme nodes. Various inequalities involving its singular values are obtained, as well as results that have applications to the convergence rate of the Conjugate Gradient method for positive definite linear systems, the minimal residual method, and the symmetric Lanczos algorithm for eigenvalue problems.

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

$$\sigma_1(X) \le \sigma_2(X) \le \cdots \le \sigma_{\min\{m,n\}}(X). \tag{1.2}$$

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

$$\kappa_{\mathrm{F}}(X) \stackrel{\mathrm{def}}{=} \sqrt{\sum_{j=1}^{\min\{m,n\}} [\sigma_j(X)]^2} \sqrt{\sum_{j=1}^{\min\{m,n\}} \frac{1}{[\sigma_j(X)]^2}}.$$

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

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 jth column. The superscript "$\cdot^*$" takes conjugate transpose while "$\cdot^T$" 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 and $i : i = \{i\}$. For vector u and matrix X, $u_{(j)}$ is u's jth entry, $X_{(i,j)}$ is X's (i,j)th entry, $\mathsf{diag}(u)$ is the diagonal matrix with $(\mathsf{diag}(u))_{(j,j)} = u_{(j)}$; X's submatrices $X_{(k:\ell,i:j)}$, $X_{(k:\ell,:)}$, and $X_{(:,i:j)}$ consists 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 smaller than ξ; while $\lceil \xi \rceil$ is the smallest integer that is larger than ξ.

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 goes to ∞. For this purpose, we shall use

> $a_n \overset{n}{\sim} b_n$ to mean that there are constants c_1, c_2, d_1, and d_2 such that $c_1 n^{d_1} \le a_n/b_n \le c_2 n^{d_2}$, and $a_n \sim b_n$ if $a_n/b_n \to 1$ as $n \to \infty$.

2 Chebyshev polynomials

The nth Chebyshev polynomial of the 1st kind is

$$\begin{aligned} T_n(t) &= \cos(n \arccos t) && \text{for } |t| \le 1, && (2.1)\\ &= \frac{1}{2}\left(t + \sqrt{t^2-1}\right)^n + \frac{1}{2}\left(t - \sqrt{t^2-1}\right)^n && \text{for } |t| \ge 1. && (2.2)\end{aligned}$$

It frequently shows up in numerical analysis and computations because of its numerous nice properties, for example $|T_n(t)| \le 1$ for $|t| \le 1$ and $|T_n(t)|$ grows extremely fast for $|t| > 1$. It is known (see, e.g., [11])

$$\left|T_n\left(\frac{1+t}{1-t}\right)\right| \equiv \left|T_n\left(\frac{t+1}{t-1}\right)\right| = \frac{1}{2}\left[\Delta_t^n + \Delta_t^{-n}\right] \quad \text{for } 1 \ne t > 0, \tag{2.3}$$

where

$$\Delta_t \stackrel{\text{def}}{=} \frac{\sqrt{t}+1}{|\sqrt{t}-1|} \quad \text{for } 1 \ne t > 0. \tag{2.4}$$

Given two (real or complex) numbers $\omega \ne 0$ and τ, the nth *Translated Chebyshev Polynomial* in x of degree n is defined by

$$\begin{aligned} T_n(x;\omega,\tau) &\stackrel{\text{def}}{=} T_n(x/\omega+\tau), && (2.5)\\ &= a_{nn}x^n + a_{n-1\,n}x^{n-1} + \cdots + a_{1n}x + a_{0n}, && (2.6) \end{aligned}$$

where $a_{jn} \equiv a_{jn}(\omega,\tau)$ are functions of ω and τ in (2.18). Their explicit dependence on ω and τ is often suppressed for convenience. Define

$$\begin{aligned} &\text{Chebyshev zero nodes:} && t_{jn} = \cos\theta_{jn},\ \theta_{jn} = \frac{2j-1}{2n}\pi,\ 1 \le j \le n, && (2.7)\\ &\text{translated Chebyshev zero nodes:} && t_{jn}^{\mathsf{tr}} = \omega(t_{jn} - \tau),\ 1 \le j \le n. && (2.8) \end{aligned}$$

It can be seen that t_{jn} $(1 \le j \le n)$ are the zeros of $T_n(t)$, while t_{jn}^{tr} $(1 \le j \le n)$ are the zeros of $T_n(x;\omega,\tau)$. Define

$$\begin{aligned} &\text{Chebyshev extreme nodes:} && \tau_{jn} = \cos\vartheta_{jn},\ \vartheta_{jn} = \frac{j}{n}\pi,\ 0 \le j \le n, && (2.9)\\ &\text{translated Chebyshev extreme nodes:} && \tau_{jn}^{\mathsf{tr}} = \omega(\tau_{jn} - \tau),\ 0 \le j \le n. && (2.10) \end{aligned}$$

τ_{jn} $(0 \le j \le n)$ are the extreme points of $T_n(t)$ on $[-1,1]$. For integer $m \ge 1$, define upper triangular $R_m \in \mathbb{C}^{m\times m}$, a matrix-valued function in ω and τ, as

$$R_m \equiv R_m(\omega,\tau) \stackrel{\text{def}}{=} \begin{pmatrix} a_{00} & a_{01} & a_{02} & \cdots & a_{0\,m-1}\\ & a_{11} & a_{12} & \cdots & a_{1\,m-1}\\ & & a_{22} & \cdots & a_{2\,m-1}\\ & & & \ddots & \vdots\\ & & & & a_{m-1\,m-1} \end{pmatrix}, \tag{2.11}$$

i.e., the jth column consists of the coefficients of $T_{j-1}(x;\omega,\tau)$. In [10], $S_{n,p}(\omega,\tau)$ is defined by

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

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

$$\begin{aligned} S_{n,1}(\omega,0) &= \frac{1}{2}\left[\left(\frac{1}{|\omega|} + \sqrt{1+\frac{1}{|\omega|^2}}\right)^n + \left(\frac{1}{|\omega|} - \sqrt{1+\frac{1}{|\omega|^2}}\right)^n\right], && (2.12)\\ &\sim \frac{1}{2}\left(\frac{1}{|\omega|} + \sqrt{1+\frac{1}{|\omega|^2}}\right)^n, && (2.13) \end{aligned}$$

and for all real τ with $|\tau| \geq 1$:

$$
\begin{aligned}
S_{n,1}(\omega,\tau) \quad = \quad & \frac{1}{2}\left[\left(\frac{1}{|\omega|}+|\tau|\right)+\sqrt{\left(\frac{1}{|\omega|}+|\tau|\right)^2-1}\right]^n \\
& +\frac{1}{2}\left[\left(\frac{1}{|\omega|}+|\tau|\right)+\sqrt{\left(\frac{1}{|\omega|}+|\tau|\right)^2-1}\right]^{-n}, \qquad (2.14) \\
\sim \quad & \frac{1}{2}\left[\left(\frac{1}{|\omega|}+|\tau|\right)+\sqrt{\left(\frac{1}{|\omega|}+|\tau|\right)^2-1}\right]^n. \qquad (2.15)
\end{aligned}
$$

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

$$
\begin{aligned}
(n+1)^{-1/p'} S_{n,1}(\omega,\tau) \leq \quad & S_{n,p}(\omega,\tau) \quad \leq S_{n,1}(\omega,\tau), \qquad (2.16) \\
\lceil (n+1)/2 \rceil^{-1/p'} S_{n,1}(\omega,0) \leq \quad & S_{n,p}(\omega,0) \quad \leq S_{n,1}(\omega,0), \qquad (2.17)
\end{aligned}
$$

where $1/p + 1/p' = 1$.

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

$$
\omega = \frac{\beta-\alpha}{2} > 0, \quad \tau = -\frac{\alpha+\beta}{\beta-\alpha}. \qquad (2.18)
$$

The linear transformation

$$
t(x) = \frac{x}{\omega} + \tau = \frac{2}{\beta-\alpha}\left(x - \frac{\alpha+\beta}{2}\right) \qquad (2.19)
$$

maps $x \in [\alpha,\beta]$ one-to-one and onto $t \in [-1,1]$. The inverse transformation is $x(t) = \omega(t-\tau)$.

3 A general lower bound for $V_{k,n}$

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 ℓ_p vector and operator norm. Given $1 \leq p \leq \infty$, the ℓ_p-norm of 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 is proved that [9] $\|X\|_p = \|X^T\|_{p'}$, where $1/p + 1/p' = 1$.

Let, throughout this paper,

$$
V_{k,n} = (V_n)_{(:,1:k)}
$$

be the submatrix of the first k rows of V_n. We define[1]

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

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

$$\mathsf{lub}_p(V_{k,n}) \le \frac{n^{1/p'}}{S_{k-1,p'}(\omega,\tau)}. \tag{3.2}$$

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

$$V_{k,n}^T v = \left(T_{k-1}(\alpha_1/\omega+\tau)\ \ T_{k-1}(\alpha_2/\omega+\tau)\ \cdots\ T_{k-1}(\alpha_n/\omega+\tau)\right)^T$$

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

$$\mathsf{lub}_p(V_{k,n}) = \min_{u\in\mathbb{R}^k} \frac{\|V_{k,n}^T u\|_{p'}}{\|u\|_{p'}} \le \frac{\|V_{k,n}^T v\|_{p'}}{\|v\|_{p'}} \le \frac{n^{1/p'}}{\left(\sum_{j=0}^{k-1} |a_{j,k-1}|^{p'}\right)^{1/p'}},$$

as expected. We have proved the following theorem.

Theorem 3.1 *For V_n with all nodes $\alpha_j \in [\alpha,\beta]$,*

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

where ω and τ are defined as in (2.18).

Theorem 3.2 *Let V_n be with all nodes $\alpha_j \in [\alpha,\beta]$, and suppose* $\max_j |\alpha_j| \ge \eta \max\{|\alpha|,|\beta|\}$ *for some $\eta > 0$.*

1. *If $-\alpha = \beta$, then*

$$\begin{aligned} \kappa_p(V_{k,n}) &\ge \max\{1, \eta^{k-1}\beta^{k-1}\} \frac{S_{k-1,1}(\beta,0)}{\lceil k/2\rceil^{1/p}\, n^{1/p'}} \qquad (3.4)\\ &\sim \frac{1}{2\lceil k/2\rceil^{1/p}\, n^{1/p'}} \times \\ &\quad \max\left\{ \left(\frac{1}{\beta} + \sqrt{1+\frac{1}{\beta^2}}\right)^{k-1}, \eta^{k-1}\left(\beta + \sqrt{1+\beta^2}\right)^{k-1} \right\}. \qquad (3.5) \end{aligned}$$

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

2. If $0 \le \alpha < \beta$*, then*

$$\begin{aligned}
\kappa_p(V_{k,n}) &\ge \max\{1, \eta^{k-1}\beta^{k-1}\}\frac{S_{k-1,1}(\omega,\tau)}{k^{1/p}\,n^{1/p'}} && (3.6)\\
&\ge \max\{1, \eta^{k-1}\beta^{k-1}\}\frac{S_{k-1,1}(\beta/2,1)}{k^{1/p}\,n^{1/p'}} && (3.7)\\
&\sim \frac{1}{2k^{1/p}\,n^{1/p'}} \times \max\left\{\left(\frac{2}{\beta}+1+2\sqrt{\frac{1}{\beta^2}+\frac{1}{\beta}}\right)^{k-1},\right.\\
&\qquad \left.\eta^{k-1}\left(2+\beta+2\sqrt{1+\beta}\right)^{k-1}\right\}. && (3.8)
\end{aligned}$$

The right-hand side of (3.7) is a lower bound for $\kappa_p(V_{k,n})$ *for* $0 = \alpha < \beta$*, too, by* Theorem 3.1.

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

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

Now if $-\alpha = \beta$, then $\omega = \beta$ and $\tau = 0$, and by (2.13) and (2.17)

$$S_{k-1,p'}(\beta,0) \ge \lceil k/2\rceil^{-1/p} S_{k-1,1}(\beta,0) \sim \lceil k/2\rceil^{-1/p}\frac{1}{2}\left(\frac{1}{\beta}+\sqrt{1+\frac{1}{\beta^2}}\right)^{k-1}.$$

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

If $0 \le \alpha < \beta$, then $\omega = (\beta-\alpha)/2 \le \beta/2$ and $\tau \le -1$. Since $S_{k-1,p'}(\omega,\tau) = S_{k-1,p'}(|\omega|,|\tau|)$ and it is increasing in $|\tau|$ and decreasing in $|\omega|$ [10], we have by (2.15) and (2.16)

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

This, together with Theorem 3.1 and (3.9), lead to (3.6) – (3.8). ∎

4 V_n with Chebyshev zero nodes

In this section, V_n has the translated Chebyshev zero nodes $\alpha_j = t_{jn}^{\mathsf{tr}}$ $(1 \le j \le n)$, except possibly those $V_{k,n}$ in Theorem 4.3. It can be proved that [11]

$$\begin{aligned}
V_n^T R_n &= \boldsymbol{T}_n \stackrel{\text{def}}{=} \begin{pmatrix} T_0(t_{1n}) & T_1(t_{1n}) & T_2(t_{1n}) & \cdots & T_{n-1}(t_{1n})\\ T_0(t_{2n}) & T_1(t_{2n}) & T_2(t_{2n}) & \cdots & T_{n-1}(t_{2n})\\ \vdots & \vdots & \vdots & & \vdots\\ T_0(t_{nn}) & T_1(t_{nn}) & T_2(t_{nn}) & \cdots & T_{n-1}(t_{nn})\end{pmatrix}, && (4.1)\\
\boldsymbol{T}_n^T\boldsymbol{T}_n &= (n/2)\,\mathsf{diag}(2,1,1,\ldots,1). && (4.2)
\end{aligned}$$

Notice that $\boldsymbol{T}_n$ is real while V_n and R_n may be complex if ω or τ is. This essentially gives a QR decomposition for V_n^T after normalizing $\boldsymbol{T}_n$'s columns to have unit norm. Extracting the first k columns from the both sides of $V_n^T = \boldsymbol{T}_n R_n^{-1}$ yields the following theorem [11].

Theorem 4.1 *Let V_n have the translated Chebyshev zero nodes $\alpha_j = t_{jn}^{\mathsf{tr}}$ $(1 \le j \le n)$, and let upper triangular R_k be defined as in* (2.11) *and $\boldsymbol{T}_n$ as in* (4.1). *Then $V_{k,n}^T = (\boldsymbol{T}_n)_{(:,1:k)}\, R_k^{-1}$.*

4.1 Condition number $\kappa_{\mathrm{F}}(V_{k,n})$

By Theorem 4.1, we have

$$\begin{aligned}
\bar V_{k,n} V_{k,n}^T &= R_k^{-*}\left[(\boldsymbol{T}_n)_{(:,1:k)}\right]^T (\boldsymbol{T}_n)_{(:,1:k)} R_k^{-1} \\
&= R_k^{-*}(\boldsymbol{T}_n^T \boldsymbol{T}_n)_{(1:k,1:k)}\, R_k^{-1} \\
&= (n/2)\, R_k^{-*}\, \mathsf{diag}(2,1,1,\ldots,1)\, R_k^{-1}, && (4.3)\\
(\bar V_{k,n} V_{k,n}^T)^{-1} &= (2/n)\, R_k\, \mathsf{diag}(2^{-1},1,1,\ldots,1)\, R_k^{*}, && (4.4)
\end{aligned}$$

where $\bar V_{k,n}$ is its complex conjugate. Consequently,

$$\begin{aligned}
\sum_j [\sigma_j(V_{k,n})]^2 &= \frac{n}{2}\,\mathrm{trace}\left(R_k^{-*}\, \mathsf{diag}(2,1,1,\ldots,1)\, R_k^{-1}\right) \\
&= \frac{n}{2}\left\|\mathsf{diag}(2^{1/2},1,1,\ldots,1)\, R_k^{-1}\right\|_{\mathrm{F}}^2, && (4.5)\\
\sum_j \frac{1}{[\sigma_j(V_{k,n})]^2} &= \frac{2}{n}\left\|\mathsf{diag}(2^{-1/2},1,1,\ldots,1)\, R_k^{*}\right\|_{\mathrm{F}}^2 \\
&= \frac{2}{n}\sum_{j=0}^{k-1}{}'\, [S_{j,2}(\omega,\tau)]^2, && (4.6)
\end{aligned}$$

where $\sum_j'$ means the first term is halved. (4.5) involves R_k^{-1}, making it a little hard to use without inverting R_k first. We might be better off by using $\sqrt{\sum_j [\sigma_j(V_{k,n})]^2} = \|V_{k,n}\|_{\mathrm{F}}$. Nevertheless it relates the singular values to the coefficients of $T_j(x;\omega,\tau)$ in a nontrivial way.

Theorem 4.2 *Let $V_{k,n}$ have the translated Chebyshev zero nodes. Then*

$$\kappa_{\mathrm{F}}(V_{k,n}) = \|V_{k,n}\|_{\mathrm{F}} \sqrt{\frac{2}{n}\sum_{j=0}^{k-1}{}'\,[S_{j,2}(\omega,\tau)]^2}.$$

Previously similar estimates (bounds) were done for $\alpha_j = t_{jn}^{\mathsf{tr}}$ on $[\alpha,\beta]$ (while $V_{k,n}$ in Theorem 4.2 may be complex) and for the following cases.

- Gautschi [6]: $k = n$, $-\alpha = \beta$ or $\alpha\beta \ge 0$, and ℓ_∞-condition number;
- Li [10]: $k = n$, $-\alpha = \beta$ or $\alpha\beta \ge 0$, and ℓ_p-condition number.

Lemma 4.1 *Let* $\alpha_j = t^{\mathsf{tr}}_{jn}$ $(1 \le j \le n)$ *on* $[\alpha, \beta]$. *Then* $\max_j |\alpha_j| = \eta \max\{|\alpha|, |\beta|\}$, *where*

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

and $\delta = \min\{|\alpha|, |\beta|\}/\max\{|\alpha|, |\beta|\} \le 1$. *Consequently for* $1 \le k \le n$

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

Proof: The expression for η is a consequence of $t^{\mathsf{tr}}_{jn} = \omega(t_{jn} - \tau) = \frac{\beta-\alpha}{2}\cos\frac{2j-1}{2n}\pi + \frac{\beta+\alpha}{2}$. The asymptotical expansion for η^{k-1} follows from expanding $(k-1)\ln\eta$ and then $\exp((k-1)\ln\eta)$. ∎

With this lemma, we have

$$\|V_{k,n}\|_{\mathrm{F}} \le \sqrt{kn}\max\{1, \max_j |t^{\mathsf{tr}}_{jn}|^{k-1}\} \sim \sqrt{kn}\,[\max\{1, |\alpha|, |\beta|\}]^{k-1}, \tag{4.7}$$

$$\|V_{k,n}\|_{\mathrm{F}} \ge \max\{1, \max_j |t^{\mathsf{tr}}_{jn}|^{k-1}\} \sim [\max\{1, |\alpha|, |\beta|\}]^{k-1}. \tag{4.8}$$

Together they imply

$$\sqrt{\sum_j [\sigma_j(V_{k,n})]^2} = \|V_{k,n}\|_{\mathrm{F}} \overset{n}{\sim} [\max\{1, |\alpha|, |\beta|\}]^{k-1}. \tag{4.9}$$

Let us now specialize Theorem 4.2 to the cases $-\alpha = \beta$ or $\alpha\beta \ge 0$. By (2.16), (4.9), and Theorem 4.2, we have

$$\kappa_{\mathrm{F}}(V_{k,n}) \overset{n}{\sim} [\max\{1, |\alpha|, |\beta|\}]^{k-1} \sum_{j=0}^{k-1} S_{j,1}(\omega, \tau). \tag{4.10}$$

First the case $-\alpha = \beta$. Then $\omega = \beta$ and $\tau = 0$. (4.10) and (2.12) yields

$$\begin{aligned} \kappa_{\mathrm{F}}(V_{k,n}) &\overset{n}{\sim} \max\{1, \beta^{k-1}\} S_{k-1,1}(\beta, 0) \\ &\overset{n}{\sim} \max\left\{ \left(\frac{1}{\beta} + \sqrt{1 + \frac{1}{\beta^2}}\right)^{k-1}, \left(\beta + \sqrt{1+\beta^2}\right)^{k-1} \right\}. \end{aligned} \tag{4.11}$$

Thus the nearly optimal conditioned $V_{k,n}$ are those with $\beta \approx 1$.

Next, consider the case $\alpha\beta \ge 0$. Without loss of generality, assume $0 \le \alpha < \beta$. (4.10) and (2.14) yields

$$\begin{aligned} \kappa_{\mathrm{F}}(V_{k,n}) &\overset{n}{\sim} \max\{1, \beta^{k-1}\} S_{k-1,1}(\omega, \tau) \\ &\ge \max\{1, \beta^{k-1}\} S_{k-1,1}(\beta/2, 1), \end{aligned} \tag{4.12}$$

and if, addition, $\alpha = 0 < \beta$,

$$\begin{aligned} \kappa_{\mathrm{F}}(V_{k,n}) &\overset{n}{\sim} \max\max\{1, \beta^{k-1}\} S_{k-1,1}(\beta/2, 1) \\ &\overset{n}{\sim} \max\left\{ \left(\frac{2}{\beta} + 1 + 2\sqrt{\frac{1}{\beta^2} + \frac{1}{\beta}}\right)^{k-1}, \left(2 + \beta + 2\sqrt{1+\beta}\right)^{k-1} \right\}. \end{aligned} \tag{4.13}$$

Thus the nearly optimal conditioned $V_{k,n}$ with $\alpha = 0 < \beta$ are also those with $\beta \approx 1$.

Since $\kappa_{\rm F} \overset{n}{\sim} \kappa_p$, all (4.11) – (4.13) for $k = n$ can be deduced from results in [10]. They, in fact, together with Theorems 3.1 and 3.2 for $k = n$ were the foundation in [10]. Now we have similar conclusions for $V_{k,n}$ with nodes in $[\alpha, \beta]$ for all k. This is summarized in the following theorem.

Theorem 4.3 *If $-\alpha = \beta$ or $\alpha\beta \geq 0$, then subject to* $(\max_j |\alpha_j|)^{n-1} \overset{n}{\sim} [\max\{|\alpha|, |\beta|\}]^{n-1}$,

$$\min \kappa_{\rm F}(V_{k,n}) \overset{n}{\sim} [\max\{1, |\alpha|, |\beta|\}]^{k-1}\, S_{k-1,1}(\omega, \tau),$$

and thus $V_{k,n}$ with $\alpha_j = t_{jn}^{\rm tr}$ $(1 \leq j \leq n)$ on $[\alpha, \beta]$ is a nearly optimally conditioned one on the interval. In particular

$$\min \kappa_{\rm F}(V_{k,n}) \overset{n}{\sim} \begin{cases} \text{RHS of (4.11)}, & \textit{for } -\alpha = \beta, \\ \text{RHS of (4.13)}, & \textit{for } 0 = \alpha < \beta. \end{cases}$$

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 [10]. 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 (4.10) were equivalent in the sense of $\overset{n}{\sim}$. 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 now. So we formulate a conjecture as follows, which has been known true for $-\alpha = \beta$ or $\alpha\beta \geq 0$, by examining (2.12) and (2.14).

Conjecture 4.1 *For $\alpha < \beta$, ω and τ defined as in* (2.18),

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

4.2 Extreme examples for CG and Lanczos

A key component in [11] for devising examples to achieve the sharpness of the existing error bounds for the Conjugate Gradient method (CG), and symmetric Lanczos method is the computation of $\min_{|u_{(1)}|=1} \|V_{k,n}^T u\|_2$ for V_n of this section. The convergence analysis of the minimal residual method (MINRES) (for $Ax = b$ with normal A) ends up with the same computation, too, except possibly complex α_j. It is proved in [11] that

$$\min_{|u_{(1)}|=1} \frac{\|V_{k,n}^T u\|_2}{\sqrt{n}} = \left[2 \sum_{j=0}^{k-1}{}' |T_j(\tau)|^2 \right]^{-1/2} \tag{4.14}$$

for $\alpha_j = t_{jn}^{\rm tr}$ on $[\alpha, \beta]$, as a consequence of (4.4). Equation (4.14), however, is valid for $\alpha_j = t_{jn}^{\rm tr}$ for any $\omega \neq 0$ and τ with or without the interval $[\alpha, \beta]$ in the context. A proof can be gotten along the same line as in [11]; see also Subsection 5.2.

4.3 Bounds on individual singular values

We start with (4.4). Let the diagonal entries of its right-hand side be d_j $(1 \le j \le k)$. Then

$$d_1 = \frac{2}{n} \sum_{i=0}^{k-1}{}' |a_{0i}|^2, \quad d_j = \frac{2}{n} \sum_{i=j-1}^{k-1} |a_{j-1\, i}|^2 \quad \text{for } 2 \le j \le k.$$

By Schur theorem [3, p.35], $\{d_j\}_{j=1}^k$ is majorized by the eigenvalues of $(\bar{V}_{k,n} V_{k,n}^T)^{-1}$ which are $\{[\sigma_j(V_{k,n})]^{-2}\}_{j=1}^k$. Recall our default ordering (1.2) on singular values to get

$$[\sigma_1(V_{k,n})]^{-2} \ge [\sigma_2(V_{k,n})]^{-2} \ge \cdots \ge [\sigma_k(V_{k,n})]^{-2}.$$

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

$$d_1^{\downarrow} \ge d_2^{\downarrow} \ge \cdots \ge d_k^{\downarrow},$$

then

$$\sum_{j=1}^{i} [\sigma_j(V_{k,n})]^{-2} \ge \sum_{j=1}^{i} d_j^{\downarrow} \quad \text{for } 1 \le i \le k \tag{4.15}$$

which can also be equivalently stated as

$$\sum_{j=i}^{k} [\sigma_j(V_{k,n})]^{-2} \le \sum_{j=i}^{k} d_j^{\downarrow} \quad \text{for } 1 \le i \le k. \tag{4.16}$$

Let us look at what we can draw from them. (4.16) implies

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

or, equivalently

$$\sigma_i(V_{k,n}) \ge \left[\sum_{j=i}^{k} d_j^{\downarrow}\right]^{-1/2} \qquad \text{for } 1 \le i \le k. \tag{4.17}$$

Take $i = 1$ in (4.15), combining with (4.17), to get for the smallest singular value

$$\left[\sum_{j=1}^{k} d_j^{\downarrow}\right]^{-1/2} \le \sigma_1(V_{k,n}) \le \left[d_1^{\downarrow}\right]^{-1/2}. \tag{4.18}$$

The lower bounds in (4.17) are guaranteed very sharp for $i = 1$ because of (4.18), but may not be so for $i \ne 1$. Our numerical calculations for various interval $[\alpha, \beta]$ shows 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., largest and smallest ones).

Exactly the same thing can be done with (4.3) upon extracting the diagonal entries of $R_k^{-*}\, \mathsf{diag}(2, 1, 1, \ldots, 1)\, R_k^{-1}$. But these diagonal entries relate to the coefficients in a much more complicated way. Detail is omitted.

5 V_n with Chebyshev extreme nodes

Since there is $n+1$ extreme points for $T_n(t)$ on $[-1,1]$, it is more convenient in terms of formula writing for us to work with V_{n+1} than V_n, and this is what we will be doing in this section. Throughout this section V_{n+1} will have nodes $\alpha_{j+1} = \tau^{\mathsf{tr}}_{jn}$ for $0 \le j \le n$. Most developments in the section resemble those in the previous section, but much more complicated computation is involved, owing to the fact that $\boldsymbol{S}_{n+1}$ below does not have orthogonal columns in contrast to $\boldsymbol{T}_n$ which does. It can be seen that

$$V_{n+1}^T R_{n+1} = \boldsymbol{S}_{n+1} \stackrel{\text{def}}{=} \begin{pmatrix} T_0(\tau_{0n}) & T_1(\tau_{0n}) & T_2(\tau_{0n}) & \cdots & T_n(\tau_{0n}) \\ T_0(\tau_{1n}) & T_1(\tau_{2n}) & T_2(\tau_{2n}) & \cdots & T_n(\tau_{2n}) \\ \vdots & \vdots & \vdots & & \vdots \\ T_0(\tau_{nn}) & T_1(\tau_{nn}) & T_2(\tau_{nn}) & \cdots & T_n(\tau_{nn}) \end{pmatrix}. \tag{5.1}$$

$\boldsymbol{S}_{n+1}$ is always real, while V_{n+1} and R_{n+1} may not. We now compute $\Upsilon_{n+1} \stackrel{\text{def}}{=} \boldsymbol{S}_{n+1}^T \boldsymbol{S}_{n+1}$. To this end, we notice

$$(\boldsymbol{S}_{n+1})_{(i+1,j+1)} = T_j(\tau_{in}) = \cos j\vartheta_{in} = \cos \frac{ji}{n}\pi,$$

and therefore for $0 \le i, j \le n$

$$\begin{aligned} (\boldsymbol{S}_n^T \boldsymbol{S}_n)_{(i+1,j+1)} &= \sum_{k=0}^{n} (\boldsymbol{S}_{n+1}^T)_{(i+1,k+1)} (\boldsymbol{S}_{n+1})_{(k+1,j+1)} \\ &= \sum_{k=0}^{n} T_i(\tau_{kn}) T_j(\tau_{kn}) \\ &= \sum_{k=0}^{n} \cos i\vartheta_{kn} \cos j\vartheta_{kn} \\ &= \frac{1}{2}\sum_{k=0}^{n} \cos(i+j)\vartheta_{kn} + \frac{1}{2}\sum_{k=0}^{n} \cos(i-j)\vartheta_{kn}. \end{aligned} \tag{5.2}$$

We now compute $\sum_{k=0}^n \cos \ell\vartheta_{kn}$, where ℓ is an integer. We claim that

$$\sum_{k=0}^{n} \cos \ell\vartheta_{kn} = \begin{cases} n+1, & \text{if } \ell = 2mn \text{ for some integer } m, \\ 0, & \text{if } \ell \text{ is odd}, \\ 1, & \text{if } \ell \text{ is even, but } \ell \ne 2mn \text{ for any integer } m. \end{cases} \tag{5.3}$$

Since $\ell\vartheta_{kn} = (\ell k/n)\pi$, the case $\ell = 2mn$ is clear. Assume that $\ell \ne 2mn$ for any integer m, and then $\cos\phi \ne 1$, where $\phi = \ell\pi/n$. Denote $\iota = \sqrt{-1}$. We have

$$\begin{aligned} 2\sum_{k=0}^{n} \cos \ell\vartheta_{kn} &= 2\sum_{k=0}^{n} \cos k\phi = \sum_{k=0}^{n} \left[e^{\iota k\phi} + e^{-\iota k\phi} \right] \\ &= \sum_{k=0}^{n} \left[e^{\iota\phi} \right]^k + \sum_{k=0}^{n} \left[e^{-\iota\phi} \right]^k \end{aligned}$$

$$
\begin{aligned}
&= \frac{1-\left[e^{\iota\phi}\right]^{n+1}}{1-e^{\iota\phi}} + \frac{1-\left[e^{-\iota\phi}\right]^{n+1}}{1-e^{-\iota\phi}} \\
&= \frac{1-e^{\iota(n+1)\phi}}{1-e^{\iota\phi}} + \frac{1-e^{-\iota(n+1)\phi}}{1-e^{-\iota\phi}} \\
&= \frac{1+\cos n\phi - \cos\phi - \cos(n+1)\phi}{1-\cos\phi} \\
&= 1+(-1)^\ell
\end{aligned}
$$

upon noticing $\cos n\phi = \cos \ell\pi = (-1)^\ell$ and $\cos(n+1)\phi = \cos(\ell\pi + \phi) = (-1)^\ell \cos\phi$. (5.3) is proved. Consider now $\ell = i \pm j$, and $0 \le i, j \le n$. Since $0 \le i+j \le 2n$ and $-n \le i-j \le n$, for some integer m

$$
\begin{aligned}
i+j = 2mn \quad &\Leftrightarrow \quad i=j=0, \quad \text{or} \quad i=j=n; \\
i-j = 2mn \quad &\Leftrightarrow \quad i=j.
\end{aligned}
$$

It follows from (5.2) and (5.3) that

$$
(\Upsilon_{n+1})_{(i+1,j+1)} = \begin{cases} n+1, & \text{for } i=j=0 \text{ or } i=j=n, \\ \frac{n}{2}+1, & \text{for } 0 \ne i = j \ne n, \\ 1, & \text{for } i \ne j, \text{ both odd or even}, \\ 0, & \text{for } i \ne j, \text{ one odd and one even}. \end{cases} \tag{5.4}
$$

Equation (5.1) yields $V_{n+1}^T = \boldsymbol{S}_{n+1} R_{n+1}^{-1}$. Extracting the first k columns from the both sides yields the following theorem.

Theorem 5.1 *Let V_{n+1} have the translated Chebyshev extreme nodes $\alpha_j = \tau_{jn}^{\mathsf{tr}}$ $(1 \le j \le n)$, and let upper triangular R_k be defined as in* (2.11) *and $\boldsymbol{S}_{n+1}$ as in* (5.1). *Then $V_{k,n+1}^T = (\boldsymbol{S}_{n+1})_{(:,1:k)} R_k^{-1}$.*

5.1 Condition number $\kappa_{\mathrm{F}}(V_{k,n+1})$

Let e_{odd} and e_{even} be two column vectors of generic dimensions[2] (i.e., determined by the context): all the odd entries of e_{odd} are ones and the even entries are zeros, and all the odd entries of e_{even} are zeros and the even entries are ones. It can be verified that

$$
\Upsilon_{n+1} = \frac{n}{2} I_{n+1} + e_{\mathsf{odd}} e_{\mathsf{odd}}^T + e_{\mathsf{even}} e_{\mathsf{even}}^T + \frac{n}{2}\left(e_1 e_1^T + e_{n+1} e_{n+1}^T\right). \tag{5.5}
$$

A rough bound for Υ_{n+1} is[3]

$$
\frac{n}{2} I_{n+1} \le \Upsilon_{n+1} \le 2n\, I_{n+1} \tag{5.6}
$$

which is probably good enough for most occasions. The left inequality is obvious and the right inequality can be proved as follows.

$$
\begin{aligned}
\|\Upsilon_{n+1}\|_2 &\le \frac{n}{2} + \|(e_{\mathsf{odd}} \quad e_{\mathsf{even}})\|_2^2 + \frac{n}{2} \\
&= n + \lceil n/2 \rceil \le 2n.
\end{aligned}
$$

[2]With generic dimensions, this is to accommodate their later use in Appendix A.

[3]$X \le Y$ for two Hermitian matrices means that $Y - X$ is positive semidefinite.

(5.6) implies immediately

$$\frac{n}{2}I_k \le (\Upsilon_{n+1})_{(1:k,1:k)} \le 2n\, I_k, \quad \frac{1}{2n}I_k \le \left[(\Upsilon_{n+1})_{(1:k,1:k)}\right]^{-1} \le \frac{2}{n}I_k \tag{5.7}$$

Better bounds will be given in Appendix A, where complicated computations are involved. For example, the upper bound in (5.6) can be improved to $n(1+\mathcal{O}(1/\sqrt{n}))I_{n+1}$ which consequently will improve inequalities in (5.7), too. But for now, we are content with what we have here for clarity. Also given in Appendix A are the quadratic form $y^*\left[(\Upsilon_{n+1})_{(1:k,1:k)}\right]^{-1}y$ that is needed for compute some CG and MINRES residuals exactly, where $y \in \mathbb{C}^k$. By Theorem 5.1, we have

$$\begin{aligned} \bar{V}_{k,n+1}V_{k,n+1}^T &= R_k^{-*}\left[(\boldsymbol{S}_{n+1})_{(:,1:k)}\right]^T(\boldsymbol{S}_{n+1})_{(:,1:k)}R_k^{-1} \\ &= R_k^{-*}\,(\boldsymbol{S}_{n+1}^T\boldsymbol{S}_{n+1})_{(1:k,1:k)}\,R_k^{-1} \\ &= R_k^{-*}\,(\Upsilon_{n+1})_{(1:k,1:k)}\,R_k^{-1}, &\quad (5.8) \\ (\bar{V}_{k,n+1}V_{k,n+1}^T)^{-1} &= R_k\,\left[(\Upsilon_{n+1})_{(1:k,1:k)}\right]^{-1}R_k^*, &\quad (5.9) \end{aligned}$$

where $\bar{V}_{k,n+1}$ is its complex conjugate. Consequently,

$$\frac{n}{2}\left\|R_k^{-1}\right\|_{\mathrm{F}}^2 \le \sum_j\left[\sigma_j(V_{k,n+1})\right]^2 \le 2n\left\|R_k^{-1}\right\|_{\mathrm{F}}^2, \tag{5.10}$$

$$\frac{1}{2n}\sum_{j=0}^{k-1}\left[S_{j,2}(\omega,\tau)\right]^2 \le \sum_j\frac{1}{\left[\sigma_j(V_{k,n+1})\right]^2} \le \frac{2}{n}\sum_{j=0}^{k-1}\left[S_{j,2}(\omega,\tau)\right]^2. \tag{5.11}$$

Theorem 5.2 *Let $V_{k,n+1}$ have the translated Chebyshev extreme nodes τ_{jn}^{tr}. Then*

$$\|V_{k,n+1}\|_{\mathrm{F}}\sqrt{\frac{1}{2n}\sum_{j=0}^{k-1}\left[S_{j,2}(\omega,\tau)\right]^2} \le \kappa_{\mathrm{F}}(V_{k,n+1}) \le \|V_{k,n+1}\|_{\mathrm{F}}\sqrt{\frac{2}{n}\sum_{j=0}^{k-1}\left[S_{j,2}(\omega,\tau)\right]^2}.$$

As what we did for Theorem 4.2, we may specialize this theorem onto interval $[\alpha,\beta]$ with the cases $-\alpha=\beta$ or $\alpha\beta\ge 0$ in an almost the same way to conclude that (4.10) – (4.13) remain true with $V_{k,n}$ there replaced by $V_{k,n+1}$ here. Detail is omitted.

5.2 Extreme examples for CG and Lanczos

V_{n+1} here provides another example to achieve the sharpness of the existing error bounds for CG, MINRES, and the symmetric Lanczos method. We shall just compute (or estimate) $\min_{|u_{(1)}|=1}\|V_{k,n+1}^Tu\|_2$ and the rest would be straightforward minor modifications to what in [11] and thus will be omitted.

Our inequalities (5.12) and (5.14) below are more general than what CG needs. They are valid, regardless whether all nodes are positive or not. It follows from a theorem in [11] that

$$\min_{|u_{(1)}|=1}\|V_{k,n+1}^Tu\|_2 = \left[e_1^T(\bar{V}_{k,n+1}V_{k,n+1}^T)^{-1}e_1\right]^{-1/2}.$$

By (5.9), we have

$$e_1^T (V_{k,n+1} V_{k,n+1}^T)^{-1} e_1 \quad = \quad y^* \, \left[(\Upsilon_{n+1})_{(1:k,1:k)} \right]^{-1} y,$$

where $y \in \mathbb{C}^k$ and $y_{(j)} = a_{0j} = T_j(\tau)$. Immediately with (5.7), we get

$$\frac{1}{\sqrt{2\Gamma_{k,\tau}}} \le \min_{|u_{(1)}|=1} \frac{\|V_{k,n+1}^T u\|_2}{\sqrt{n}} \le \sqrt{\frac{2}{\Gamma_{k,\tau}}}. \tag{5.12}$$

where

$$\Gamma_{k,\tau} \stackrel{\text{def}}{=} \sum_{j=0}^{k-1} |T_j(\tau)|^2. \tag{5.13}$$

Notice that in Appendix A, exact expressions for $y^* \, \left[(\Upsilon_{n+1})_{(1:k,1:k)} \right]^{-1} y$ are given. They will yield exact, but complicated, $\min_{|u_{(1)}|=1} \|V_{k,n+1}^T u\|_2$. In terms of studying sharpness for the existing CG and Lanczos error bounds, (5.12) is good enough. So we omit giving out the exact optimal values here. Now for a given $g \in \mathbb{C}^{n+1}$, we have

$$\frac{\sqrt{n}\,\min_j |g_{(j)}|}{\|g\|_2} \frac{1}{\sqrt{2\Gamma_{k,\tau}}} \le \min_{|u_{(1)}|=1} \frac{\|\mathsf{diag}(g)\, V_{k,n+1}^T u\|_2}{\|g\|_2} \le \frac{\sqrt{n}\,\max_j |g_{(j)}|}{\|g\|_2} \sqrt{\frac{2}{\Gamma_{k,\tau}}}. \tag{5.14}$$

(5.12) and (5.14) are valid for $\alpha_{j+1} = \tau_{jn}^{\mathsf{tr}}$ for $0 \le j \le n$ for any $\omega \ne 0$ and τ with or without the interval $[\alpha, \beta]$ in the context.

Meinardus [12] showed that *if* $0 < \alpha < \beta$, *and* $g \in \mathbb{C}^{n+1}$ *with*

$$g_{(j+1)} = \begin{cases} \sqrt{1/\tau_{jn}^{\mathsf{tr}}}, & \textit{for } j \in \{0, n\}, \\ \sqrt{2/\tau_{jn}^{\mathsf{tr}}}, & \textit{for } 1 \le j \le n-1, \end{cases} \tag{5.15}$$

then

$$\min_{|u_{(1)}|=1} \frac{\|\mathsf{diag}(g) V_{n+1}^T u\|_2}{\|g\|_2} = 2 \left[\Delta_\delta^n + \Delta_\delta^{-n} \right]^{-1}, \tag{5.16}$$

where $\delta = \alpha/\beta$ *and* Δ_δ *is defined by* (2.4). This is not exactly the way Meinardus [12] stated, but an equivalent form. Note that $V_{n+1} \equiv V_{k,n+1}$ for $k = n+1$; so the left-hand side of (5.16) is nothing but

$$\min_{|u_{(1)}|=1} \frac{\|\mathsf{diag}(g) V_{k,n+1}^T u\|_2}{\|g\|_2} \quad \text{for } k = n+1 \text{ and } g \text{ as in (5.15).}$$

Numerical tests indicate that for $1 \le k \le n$

$$\min_{|u_{(1)}|=1} \frac{\|\mathsf{diag}(g) V_{k,n+1}^T u\|_2}{\|g\|_2} < 2 \left[\Delta_\delta^{k-1} + \Delta_\delta^{-(k-1)} \right]^{-1}.$$

Our (5.14) can lead to a lower and a upper bound (for all k) that differ by at most a factor of $2\sqrt{2\beta/\alpha}$ because $\min_j |g_{(j)}| \ge 1/\sqrt{\beta}$ and $\max_j |g_{(j)}| \ge \sqrt{2/\alpha}$. For comparison purpose, let cite the following restatement of a result also due to Meinardus [12]: *If all* $\alpha_j \in [\alpha, \beta]$

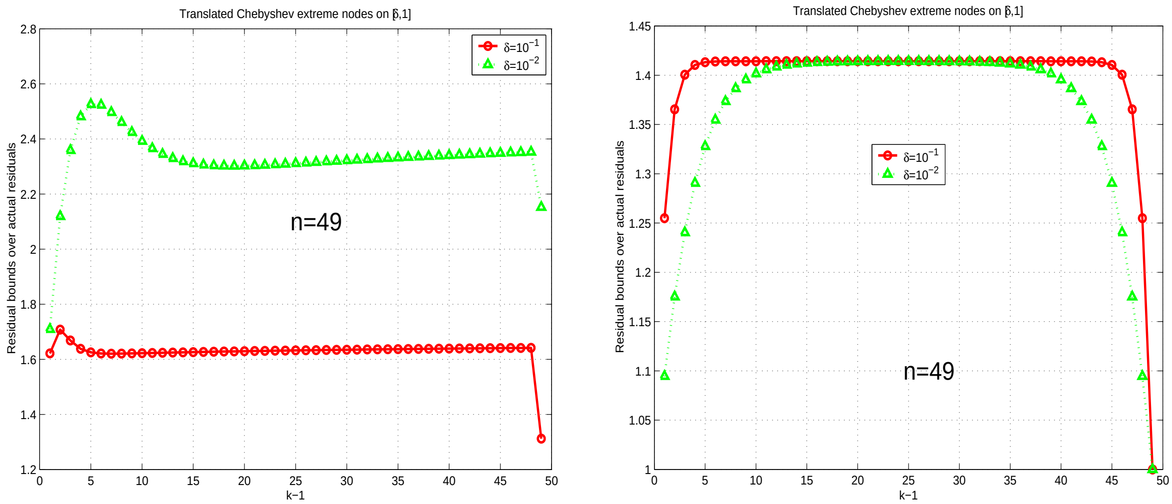

Figure 5.1: Ratios of $2\left[\Delta_\Delta^{k-1}+\Delta_\delta^{-(k-1)}\right]^{-1}$ over $\min_{|u_{(1)}|=1}\frac{\|\mathsf{diag}(g)V_{k,n+1}^T u\|_2}{\|g\|_2}$, where $\alpha_{j+1}=\tau_{jn}^{\mathsf{tr}}$ on $[\delta,1]$. **Left:** $g_{(j)}=1$ for $1\le j\le n+1$; **Right:** g defined by (5.15).

(not necessarily the translated Chebyshev extreme nodes, of course) and $0<\alpha$, *then for any* $g\in\mathbb{C}^{n+1}$,

$$\min_{|u_{(1)}|=1}\frac{\|\mathsf{diag}(g)V_{k,n+1}^T u\|_2}{\|g\|_2}\le 2\left[\Delta_\delta^{k-1}+\Delta_\delta^{-(k-1)}\right]^{-1} \tag{5.17}$$

for all $1\le k\le n+1$. Figure 5.1 plots the ratio of the right-hand side of (5.17) over its left-hand side for $\alpha_{j+1}=\tau_{jn}^{\mathsf{tr}}$ on $[\delta,1]$ with two different g. It is interesting to notice a sudden drop at $k-1=n$ for g being the vector of all ones, and for g as in (5.15), the ratio is one at $k-1=n$ guaranteed by (5.16) and for all other k the ratios appear no bigger than $\sqrt{2}$. So we put forward the following conjecture.

Conjecture 5.1 *The ratio of* $2\left[\Delta_\delta^{k-1}+\Delta_\delta^{-(k-1)}\right]^{-1}$ *over* $\min_{|u_{(1)}|=1}\frac{\|\mathsf{diag}(g)V_{k,n+1}^T u\|_2}{\|g\|_2}$ *is no bigger than* $\sqrt{2}$, *if* $\alpha_{j+1}=\tau_{jn}^{\mathsf{tr}}\in[\alpha,\beta]$ *with* $0<\alpha$ *and* g *defined by* (5.15).

5.3 Bounds on individual singular values

Let the diagonal entries of $R_kR_k^*$ be

$$\delta_j=e_j^TR_kR_k^*e_j=\sum_{i=j-1}^{k-1}|a_{j-1\,i}|^2 \quad \text{for } 1\le j\le k,$$

and the diagonal entries of $R_k\,\left[(\Upsilon_{n+1})_{(1:k,1:k)}\right]^{-1}R_k^*$ be $\tilde\delta_j$ $(1\le j\le k)$. Then by (5.7)

$$\frac{1}{2n}\delta_j\le\tilde\delta_j=e_j^TR_k\,\left[(\Upsilon_{n+1})_{(1:k,1:k)}\right]^{-1}R_k^*e_j^T\le\frac{2}{n}e_j^TR_kR_k^*e_j^T=\frac{2}{n}\delta_j.$$

Let the nonincreasing re-ordering of δ_j's and $\tilde\delta_j$'s be $\delta_j^\downarrow$'s and $\tilde\delta_j^\downarrow$'s, respectively, i.e.,

$$\delta_j^\downarrow\ge\delta_j^\downarrow\ge\cdots\ge\delta_j^\downarrow,\quad \tilde\delta_j^\downarrow\ge\tilde\delta_j^\downarrow\ge\cdots\ge\tilde\delta_j^\downarrow.$$

Equation (5.9) implies, by Schur theorem [3, p.35],

$$\sum_{j=1}^{i} [\sigma_j(V_{k,n+1})]^{-2} \quad \geq \quad \sum_{j=1}^{i} \tilde{\delta}_j^{\downarrow} \geq \frac{1}{2n} \sum_{j=1}^{i} \delta_j^{\downarrow} \quad \text{for } 1 \leq i \leq k, \tag{5.18}$$

$$\sum_{j=i}^{k} [\sigma_j(V_{k,n+1})]^{-2} \quad \leq \quad \sum_{j=i}^{k} \tilde{\delta}_j^{\downarrow} \leq \frac{2}{n} \sum_{j=i}^{k} \delta_j^{\downarrow} \quad \text{for } 1 \leq i \leq k. \tag{5.19}$$

Now (5.19) implies

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

or, equivalently

$$\sigma_i(V_{k,n+1}) \geq \sqrt{\frac{n}{2}} \left[\sum_{j=i}^{k} \delta_j^{\downarrow} \right]^{-1/2} \qquad \text{for } 1 \leq i \leq k. \tag{5.20}$$

Take $i = 1$ in (5.18), combining with (5.20), to get for the smallest singular value

$$\sqrt{\frac{n}{2}} \left[\sum_{j=1}^{k} \delta_j^{\downarrow} \right]^{-1/2} \leq \sigma_1(V_{k,n+1}) \leq \sqrt{2n} \left[\delta_1^{\downarrow} \right]^{-1/2}. \tag{5.21}$$

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

6 V_n with other orthogonal polynomial zero nodes

Part of the material in Section 4 can naturally be extended to V_n whose nodes are the zeros of the nth translated orthogonal polynomial from any orthogonal polynomial system. We shall outline the detail here. Let $p_j(t)$, $j = 0, 1, 2, \ldots$, denote a sequence of *normalized* orthogonal polynomial 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_n we have been dealing with so far, Legendre polynomials, and etc, the reader is referred to [4, p.57] or any books on orthogonal polynomials. Orthogonal polynomials have many beautiful properties. Useful to us here are that $p_n(t)$ is guaranteed to have exact n distinct zeros[4] t_{jn}, $j = 1, 2, \cdots, n$, in the interval, and [7]

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

as the result of the fact that the Gaussian quadrature formula

$$\int \phi(t)\, w(t) dt \approx \sum_{j=1}^{n} \lambda_{jn} \phi(t_{jn})$$

[4] Up to now, t_{jn} is reserved for the zeros of the nth Chebyshev polynomial of the first kind. It, along with other previously reserved notation, will be reassigned in this section.

is exact for all polynomials of degree no higher than $2n-1$ and $\int p_r(t)p_s(t)\,w(t)dt = 0$ for $r \neq s$ and 1 for $r = s$, where the integral is taken over the support of $w(t)$, λ_{jn} are Christoffel numbers for p_n. For numerical values of the nodes and Christoffel numbers for various orthgonal polynomials, the reader is referred to [1].

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

$$\begin{aligned} p_n(x;\omega,\tau) &\stackrel{\rm def}{=} p_n(x/\omega+\tau), \\ &= a_{nn}x^n + a_{n-1\,n}x^{n-1} + \cdots + a_{1n}x + a_{0n}, \end{aligned}$$

whose zeros are

$$t_{jn}^{\sf tr} = \omega(t_{jn}-\tau), \quad 1 \le j \le n.$$

Let V_n be with $\alpha_j = t_{jn}^{\sf tr}$ and set R_n as in (2.11) but with a_{ij} here. We have

$$V_n^T R_n = \boldsymbol{P}_n \stackrel{\rm def}{=} \begin{pmatrix} p_0(t_{1n}) & p_1(t_{1n}) & p_2(t_{1n}) & \cdots & p_{n-1}(t_{1n}) \\ p_0(t_{2n}) & p_1(t_{2n}) & p_2(t_{2n}) & \cdots & p_{n-1}(t_{2n}) \\ \vdots & \vdots & \vdots & & \vdots \\ p_0(t_{nn}) & p_1(t_{nn}) & p_2(t_{nn}) & \cdots & p_{n-1}(t_{nn}) \end{pmatrix}, \tag{6.2}$$

$$\boldsymbol{P}_n^T \Lambda_n \boldsymbol{P}_n = {\sf diag}(1,1,1,\ldots,1), \tag{6.3}$$

where $\Lambda_n = (\lambda_{1n},\lambda_{2n},\ldots,\lambda_{nn})$. Therefore $V_n^T = \boldsymbol{P}_n R_n^{-1}$. Extracting the first k columns from the both sides of $V_n^T = \boldsymbol{T}_n R_n^{-1}$ yields $V_{k,n}^T = (\boldsymbol{P}_n)_{(:,1:k)}\, R_k^{-1}$, similar to Theorems 4.1.

Let $\Lambda_{k,n} = (\Lambda_n)_{(1:k,1:k)}$. We have

$$\begin{aligned} \bar V_{k,n}\Lambda_{k,n}V_{k,n}^T &= R_k^{-*}\left[(\boldsymbol{P}_n)_{(:,1:k)}\right]^T \Lambda_{k,n}(\boldsymbol{P}_n)_{(:,1:k)}R_k^{-1} \\ &= R_k^{-*}(\boldsymbol{P}_n^T\Lambda_n\boldsymbol{P}_n)_{(1:k,1:k)}\,R_k^{-1} \\ &= R_k^{-*}R_k^{-1}, \qquad (6.4)\\ (\bar V_{k,n}\Lambda_{k,n}V_{k,n}^T)^{-1} &= R_kR_k^*. \qquad (6.5) \end{aligned}$$

Upon noticing $\min_j \lambda_{jn} I_k \le \Lambda_{k,n} \le \max_j \lambda_{jn} I_k$, we have

$$\frac{1}{\max_j \lambda_{jn}}\left\|R_k^{-1}\right\|_{\rm F}^2 \le \sum_j [\sigma_j(V_{k,n})]^2 \le \frac{1}{\min_j \lambda_{jn}}\left\|R_k^{-1}\right\|_{\rm F}^2, \tag{6.6}$$

$$\min_j \lambda_{jn}\,\Phi_k \le \sum_j \frac{1}{[\sigma_j(V_{k,n})]^2} \le \max_j \lambda_{jn}\,\Phi_k. \tag{6.7}$$

where

$$\Phi_k \stackrel{\rm def}{=} \|R_k\|_{\rm F}^2 = \sum_{j=0}^{k-1}\sum_{i=0}^{j} a_{ij}^2.$$

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

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

where $g = (\sqrt{\lambda_{1n}},\sqrt{\lambda_{2n}},\ldots,\sqrt{\lambda_{nn}}\,)^T$. We may also get bounds on individual singular value $\sigma_j(V_{k,n})$, following the lines of previous sections. For 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 individual singular value.

It turns out that the simple QR decompsotion for V_n with translated Chebyshev zero nodes is shared by a much large class of V_n, i.e., those with nodes being translated zeros of any orthogonal polynomials. Consequently we can get about the same things as we did 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 nearly optimal conditioned real *rectangular* Vandermonde matrices on a given interval. Previously similar results were obtained for real *square* Vandermonde matrices in [2, 10]. The second application is its implication to the convergence of the Conjugate Gradient method for positive definite linear systems and the symmetric Lanczos algorithm for symmetric eigenvalue problems. It is observed that superlinear convergence [8, 13, 14] often occur for the two methods; while existing error bounds only guaranteed linear convergence. But little study has been done as to the sharpness of the existing error bounds. Results in this paper can be used to construct examples as in [11] for which errors of approximations by both methods are comparable to the existing error bounds at all iteration steps.

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Appendix

A $(\Upsilon_{n+1})_{(1:k,1:k)}$ and its inverse

$(\Upsilon_{n+1})_{(1:k,1:k)}$ is defined in Section 5. We shall do two things here:

- to bound $(\Upsilon_{n+1})_{(1:k,1:k)}$ from above and below by scalar multiples of I_k, more sharply than in (5.7);
- to compute exactly the quadratic form $y^* \left[(\Upsilon_{n+1})_{(1:k,1:k)}\right]^{-1} y$, instead of estimates by the fairly sharp lower and upper bounds used to get (5.12).

The former will lead to lower and upper bounds on $\left[(\Upsilon_{n+1})_{(1:k,1:k)}\right]^{-1}$, too. The latter gives exact residual errors for CG and MINRES on certain linear systems.

The case for small n, i.e., $1 \le n \le 3$, can be easily exhausted. In fact, we have

$$\Upsilon_{1+1} = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}, \ \Upsilon_{2+1} = \begin{pmatrix} 3 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 3 \end{pmatrix}, \ \Upsilon_{3+1} = \begin{pmatrix} 4 & 0 & 1 & 0 \\ 0 & 5/2 & 0 & 1 \\ 1 & 0 & 5/2 & 0 \\ 0 & 1 & 0 & 4 \end{pmatrix}.$$

So we shall assume $n \ge 4$ from now on. Denote

$$k_2^+ \stackrel{\text{def}}{=} \lceil k/2 \rceil, \quad k_2^- \stackrel{\text{def}}{=} \lfloor k/2 \rfloor. \tag{A.1}$$

For $y \in \mathbb{C}^k$, set

$$y_{\mathsf{odd}} = \sum_{\text{odd } i} y_{(i)}, \quad y_{\mathsf{even}} = \sum_{\text{even } i} y_{(i)}. \tag{A.2}$$

A.1 The case $k \le 2$

There is not much to say about $k = 1$ since $(\Upsilon_{n+1})_{(1,1)} = n + 1$, a scalar. For $k = 2$,

$$(\Upsilon_{n+1})_{(1:2,1:2)} = \begin{pmatrix} n+1 & 0 \\ 0 & \frac{n}{2}+1 \end{pmatrix}.$$

A.2 The case $3 \le k < n + 1$

We have

$$\begin{aligned}(\Upsilon_{n+1})_{(1:k,1:k)} &= \frac{n}{2} I_k + e_{\mathsf{odd}} e_{\mathsf{odd}}^T + e_{\mathsf{even}} e_{\mathsf{even}}^T + \frac{n}{2} e_1 e_1^T \\ &= \frac{n}{2}\left[I_k + (e_1 \ \zeta e_{\mathsf{odd}} \ \zeta e_{\mathsf{even}})(e_1 \ \zeta e_{\mathsf{odd}} \ \zeta e_{\mathsf{even}})^T\right] \\ &= \frac{n}{2}(I_k + W_{3e} W_{3e}^T), \end{aligned} \tag{A.3}$$

where

$$\zeta = \sqrt{2/n}, \quad W_{3e} = (e_1 \ \zeta e_{\mathsf{odd}} \ \zeta e_{\mathsf{even}}). \tag{A.4}$$

We use Sherman-Morrison-Woodbury formula [5, p.95] to find its inverse:

$$(I_k + W_{3e} W_{3e}^T)^{-1} = I - W_{3e}(I + W_{3e}^T W_{3e})^{-1} W_{3e}^T. \tag{A.5}$$

Noticing $e_{\mathsf{odd}}^T e_{\mathsf{odd}} = k_2^+$ and $e_{\mathsf{even}}^T e_{\mathsf{even}} = k_2^-$, we have

$$W_{3e}^T W_{3e} = \begin{pmatrix} 1 & \zeta & 0 \\ \zeta & \zeta^2 k_2^+ & 0 \\ 0 & 0 & \zeta^2 k_2^- \end{pmatrix}$$

whose eigenvalues are

$$\lambda_1 = \frac{2k_2^-}{n}, \quad \lambda_2 = \frac{n + 2k_2^+ + \sqrt{\xi}}{2n}, \quad \lambda_3 = \frac{n + 2k_2^+ - \sqrt{\xi}}{2n},$$

where $\xi = n^2 - 4nk_2^+ + 4(k_2^+)^2 + 8n$. It can be proved that λ_2 and λ_3 increase as k_2^+ does, and thus with the help of $2 \le k_2^+ \le \frac{n+1}{2}$ and $1 \le k_2^- \le \frac{n}{2}$, we have

$$\begin{aligned} \frac{2}{n} \le \ &\lambda_1 \le 1, \\ \frac{n+4+\sqrt{n^2+16}}{2n} \le \ &\lambda_2 \le \frac{2n+1+\sqrt{8n+1}}{2n}, \\ \frac{n+4-\sqrt{n^2+16}}{2n} \le \ &\lambda_3 \le \frac{2n+1-\sqrt{8n+1}}{2n}. \end{aligned}$$

With which, we deduce that

$$\frac{n}{2}\left(1 + \frac{n+4-\sqrt{n^2+16}}{2n}\right) I_k \le (\Upsilon_{n+1})_{(1:k,1:k)} \le \frac{n}{2}\left(1 + \frac{2n+1+\sqrt{8n+1}}{2n}\right) I_k. \tag{A.6}$$

Next, we compute the quadratic form $y^*\left[(\Upsilon_{n+1})_{(1:k,1:k)}\right]^{-1}y$. We will use (A.5) and

$$I + W_{3e}^T W_{3e} \;=\; I + \begin{pmatrix} 1 & \zeta & 0 \\ \zeta & \zeta^2 k_2^+ & 0 \\ 0 & 0 & \zeta^2 k_2^- \end{pmatrix}, \tag{A.7}$$

$$(I + W_{3e}^T W_{3e})^{-1} \;=\; \begin{pmatrix} \frac{\zeta^2 k_2^+ + 1}{c} & -\frac{\zeta}{c} & 0 \\ -\frac{\zeta}{c} & \frac{2}{c} & 0 \\ 0 & 0 & \frac{1}{1+\zeta^2 k_2^-} \end{pmatrix}, \tag{A.8}$$

where $c = (2k_2^+ - 1)\zeta^2 + 2 = (2\lceil k/2\rceil - 1)\frac{2}{n} + 2$. Then

$$\begin{aligned} y^* W_{3e} &= \begin{pmatrix} y_{(1)} & \zeta y_{\mathsf{odd}} & \zeta y_{\mathsf{even}} \end{pmatrix}, \\ \frac{n}{2} y^*\left[(\Upsilon_{n+1})_{(1:k,1:k)}\right]^{-1} y &= y^* y - \left[\frac{\zeta^2 k_2^+ + 1}{c} |y_{(1)}|^2 - \frac{2\zeta^2}{c} \mathrm{R\scriptstyle E}\left(y_{(1)} y_{\mathsf{odd}}\right)\right. \\ &\quad \left. + \frac{2\zeta^2}{c} |y_{\mathsf{odd}}|^2 + \frac{\zeta^2}{1+\zeta^2 k_2^-} |y_{\mathsf{even}}|^2\right], \\ y^*\left[(\Upsilon_{n+1})_{(1:k,1:k)}\right]^{-1} y &= \frac{2}{n} y^* y - \left[\frac{2(2\lceil k/2\rceil + n)}{cn^2} |y_{(1)}|^2 - \frac{8}{cn^2} \mathrm{R\scriptstyle E}\left(y_{(1)} y_{\mathsf{odd}}\right)\right. \\ &\quad \left. + \frac{8}{cn^2} |y_{\mathsf{odd}}|^2 + \frac{4}{n(n+2\lfloor k/2\rfloor)} |y_{\mathsf{even}}|^2\right], \end{aligned} \tag{A.9}$$

where $\mathrm{R\scriptstyle E}(\cdot)$ takes the real part of a complex number.

A.3 The case $k = n + 1$

Now it is Υ_{n+1} itself. Similarly

$$\begin{aligned} \Upsilon_{n+1} &= \frac{n}{2}(I_k + W_{4e} W_{4e}^T), \\ [\Upsilon_{n+1}]^{-1} &= \frac{2}{n}\left(I - W_{4e}(I + W_{4e}^T W_{4e})^{-1} W_{4e}^T\right), \end{aligned} \tag{A.10}$$

where

$$\zeta = \sqrt{2/n}, \quad W_{4e} = (e_1 \;\, \zeta e_{\mathsf{odd}} \;\, e_{n+1} \;\, \zeta e_{\mathsf{even}}). \tag{A.11}$$

Equation (A.5) remains true with W_{3e} replaced by W_{4e}. But $I_4 + W_{4e}^T W_{4e}$ takes different forms, depending on oddity of $n + 1$.

The case $k = n + 1$ and is odd. Now $k_2^+ = (n + 2)/2$ and $k_2^- = n/2$. It can be verified that

$$W_{4e}^T W_{4e} = \begin{pmatrix} 1 & \zeta & 0 & 0 \\ \zeta & \zeta^2 k_2^+ & \zeta & 0 \\ 0 & \zeta & 1 & 0 \\ 0 & 0 & 0 & \zeta^2 k_2^- \end{pmatrix}$$

whose eigenvalues are

$$\frac{2n + 2 - 2\sqrt{4n+1}}{2n}, \quad 1, \quad 1, \quad \frac{2n + 2 + 2\sqrt{4n+1}}{2n}.$$

With which, we deduce that

$$\frac{n}{2}\left(1+\frac{2n+2-2\sqrt{4n+1}}{2n}\right)I_{n+1}\leq\Upsilon_{n+1}\leq\frac{n}{2}\left(1+\frac{2n+2+2\sqrt{4n+1}}{2n}\right)I_{n+1}. \qquad \text{(A.12)}$$

Next, we compute the quadratic form $y^*\left[\Upsilon_{n+1}\right]^{-1}y$. We will use (A.10) and

$$\begin{aligned}
I+W_{4e}^TW_{4e} &= \begin{pmatrix} 2 & \sqrt{\frac{2}{n}} & 0 & 0\\ \sqrt{\frac{2}{n}} & \frac{2(n+1)}{n} & \sqrt{\frac{2}{n}} & 0\\ 0 & \sqrt{\frac{2}{n}} & 2 & 0\\ 0 & 0 & 0 & 2\end{pmatrix},\\
(I+W_{4e}^TW_{4e})^{-1} &= \begin{pmatrix} \frac{2n+1}{4n} & -\frac{1}{2\sqrt{2n}} & \frac{1}{4n} & 0\\ -\frac{1}{2\sqrt{2n}} & \frac{1}{2} & -\frac{1}{2\sqrt{2n}} & 0\\ \frac{1}{4n} & -\frac{1}{2\sqrt{2n}} & \frac{2n+1}{4n} & 0\\ 0 & 0 & 0 & \frac{1}{2}\end{pmatrix}.
\end{aligned}$$

Consequently

$$\begin{aligned}
y^*W_{4e} &= \begin{pmatrix} y_{(1)} & \zeta y_{\mathsf{odd}} & y_{(n+1)} & \zeta y_{\mathsf{even}}\end{pmatrix}, \qquad \text{(A.13)}\\
\frac{n}{2}y^*\Upsilon_{n+1}^{-1}y &= y^*y-\left[\frac{2n+1}{4n}|y_{(1)}|^2+\frac{1}{2}\zeta^2|y_{\mathsf{odd}}|^2+\frac{2n+1}{4n}|y_{(n+1)}|^2\right.\\
&\quad -\frac{1}{\sqrt{2n}}\zeta\mathrm{R}\textsc{e}\left(y_{(1)}y_{\mathsf{odd}}\right)+\frac{1}{2n}\mathrm{R}\textsc{e}\left(y_{(1)}y_{(n+1)}\right)-\frac{1}{\sqrt{2n}}\zeta\mathrm{R}\textsc{e}\left(y_{(n+1)}y_{\mathsf{odd}}\right)\\
&\quad \left.+\frac{1}{2}\zeta^2|y_{\mathsf{even}}|^2\right],\\
y^*\Upsilon_{n+1}^{-1}y &= \frac{2}{n}y^*y-\frac{2}{n}\left[\frac{2n+1}{4n}|y_{(1)}|^2+\frac{1}{n}|y_{\mathsf{odd}}|^2+\frac{2n+1}{4n}|y_{(n+1)}|^2\right.\\
&\quad -\frac{1}{n}\mathrm{R}\textsc{e}\left(y_{(1)}y_{\mathsf{odd}}\right)+\frac{1}{2n}\mathrm{R}\textsc{e}\left(y_{(1)}y_{(n+1)}\right)-\frac{1}{n}\mathrm{R}\textsc{e}\left(y_{(n+1)}y_{\mathsf{odd}}\right)\\
&\quad \left.+\frac{1}{n}|y_{\mathsf{even}}|^2\right]. \qquad \text{(A.14)}
\end{aligned}$$

The case $k=n+1$ and is even. Now $k_2^+=(n+1)/2$ and $k_2^-=(n+1)/2$. It can be verified that

$$W_{4e}^TW_{4e}=\begin{pmatrix}1 & \zeta & 0 & 0\\ \zeta & \zeta^2k_2^+ & 0 & 0\\ 0 & 0 & 1 & \zeta\\ 0 & 0 & \zeta & \zeta^2k_2^-\end{pmatrix}$$

whose eigenvalues are two copies of

$$\frac{2n+1-\sqrt{8n+1}}{2n},\quad \frac{2n+1+\sqrt{8n+1}}{2n}.$$

With which, we deduce that

$$\frac{n}{2}\left(1+\frac{2n+1-\sqrt{8n+1}}{2n}\right)I_{n+1} \le \Upsilon_{n+1} \le \frac{n}{2}\left(1+\frac{2n+1+\sqrt{8n+1}}{2n}\right)I_{n+1}. \tag{A.15}$$

Next, we compute the quadratic form $y^*\left[\Upsilon_{n+1}\right]^{-1}y$. We will use (A.10) and

$$\begin{aligned} I+W_{4e}^TW_{4e} &= \begin{pmatrix} 2 & \sqrt{\frac{2}{n}} & 0 & 0 \\ \sqrt{\frac{2}{n}} & \frac{2n+1}{n} & 0 & 0 \\ 0 & 0 & 2 & \sqrt{\frac{2}{n}} \\ 0 & 0 & \sqrt{\frac{2}{n}} & \frac{2n+1}{n} \end{pmatrix}, \\ (I+W_{4e}^TW_{4e})^{-1} &= \begin{pmatrix} \frac{2n+1}{4n} & -\frac{1}{2\sqrt{2n}} & 0 & 0 \\ -\frac{1}{2\sqrt{2n}} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{2n+1}{4n} & -\frac{1}{2\sqrt{2n}} \\ 0 & 0 & -\frac{1}{2\sqrt{2n}} & \frac{1}{2} \end{pmatrix}. \end{aligned}$$

Consequently, we have (A.13) and

$$\begin{aligned} \frac{n}{2}y^*\Upsilon_{n+1}^{-1}y &= y^*y-\left[\frac{2n+1}{4n}\left(|y_{(1)}|^2+|y_{(n+1)}|^2\right)+\frac{1}{2}\zeta^2\left(|y_{\mathsf{odd}}|^2+|y_{\mathsf{even}}|^2\right)\right. \\ &\quad \left.-\frac{1}{\sqrt{2n}}\zeta\left(\mathrm{R}\text{E}\left(y_{(1)}y_{\mathsf{odd}}\right)+\mathrm{R}\text{E}\left(y_{(n+1)}y_{\mathsf{even}}\right)\right)\right], \\ y^*\Upsilon_{n+1}^{-1}y &= \frac{2}{n}y^*y-\frac{2}{n}\left[\frac{2n+1}{4n}\left(|y_{(1)}|^2+|y_{(n+1)}|^2\right)+\frac{1}{n}\left(|y_{\mathsf{odd}}|^2+|y_{\mathsf{even}}|^2\right)\right. \\ &\quad \left.-\frac{1}{n}\left(\mathrm{R}\text{E}\left(y_{(1)}y_{\mathsf{odd}}\right)+\mathrm{R}\text{E}\left(y_{(n+1)}y_{\mathsf{even}}\right)\right)\right]. \end{aligned} \tag{A.16}$$