Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 39, pp. 572-590, November 2023.

SHELL EXTREMAL EIGENVALUES OF TRIDIAGONAL TOEPLITZ MATRICES*

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Abstract. The shell of a complex tridiagonal Toeplitz matrix is studied. Closed formulas for all quantities involved in its equation are presented. Necessary and sufficient conditions for a Toeplitz tridiagonal matrix to have shell extremal eigenvalues are given. Several, recently introduced, geometric quantities related to the shell are studied as measures of non-normality of these extremal eigenvalues of such matrices. These quantities are also proposed as measures of non-normality for the matrix itself.

Key words. Shell, Cubic curve, Toeplitz matrix, Extremal eigenvalues, Non-normal matrix.

AMS subject classifications. 15A18, 15A60, 15B05, 15B57.

1. Introduction and preliminaries. Let $\mathbb{C}$ be the complex field. For $a \in \mathbb{C}$, we denote by $\mathrm{Re}\{a\}$ and $\mathrm{Im}\{a\}$ the real and imaginary parts of a, respectively. $M_n(\mathbb{C})$ is the vector space of $n \times n$ complex matrices. For $A \in M_n(\mathbb{C})$, $H(A) = \dfrac{A + A^*}{2}$ and $K(A) = \dfrac{A - A^*}{2}$ are the hermitian and skew-hermitian parts of A, respectively. We denote by $\delta_i(A),\ i = 1, \cdots, n$ the eigenvalues of $H(A)$ in decreasing order and by $\mathbf{y}_i$ their corresponding eigenvectors. Let also $u(A) = \mathrm{Im}\{\mathbf{y}_1^* K(A)\mathbf{y}_1\}$ and $\nu(A) = \|K(A)\mathbf{y}_1\|_2^2$, where $\|\cdot\|_2$ denotes the euclidean norm. The standard numerical range $F(A)$ of a square matrix A is the set of quadratic forms $\mathbf{x}^* A\mathbf{x}$, where the complex n dimensional vectors $\mathbf{x}$ are of euclidean norm one (see Chapter 1 in [11]).

The shell of a square matrix A [2] is the cubic curve $\Gamma(A)$ defined as

$$\Gamma(A) = \{z = x + \mathrm{i}y, x, y \in \mathbb{R} : g_A(x, y) = 0\}, \tag{1.1}$$

$$g_A(x, y) = [(\delta_1(A) - x)^2 + (u(A) - y)^2](\delta_2(A) - x) + (\delta_1(A) - x)(\nu(A) - u(A)^2). \tag{1.2}$$

The curve $\Gamma(A)$ is symmetric with respect to the horizontal line $\ell = \{t + \mathrm{i}u(A), t \in \mathbb{R}\}$ and provides interesting spectral localization results. In fact for every eigenvalue λ of A it holds that $\lambda \in \Gamma_{in}(A)$, where $\Gamma_{in}(A) = \{z = x + \mathrm{i}y, x, y \in \mathbb{R} : g_A(x, y) \geq 0\}$. Much of this analysis is based on the sign of the discriminant $D(A) = (\delta_1(A) - \delta_2(A))^2 - 4(\nu(A) - u(A)^2)$. Specifically, when $D(A) < 0$, then $\Gamma(A)$ is a simple unbounded open curve that leaves all eigenvalues of A to its left. When $D(A) = 0$, it creates a node point and when $D(A) > 0$ it consists of two branches, a closed branch (loop) that surrounds a unique simple eigenvalue and an open branch that has all its remaining eigenvalues to its left. Note that $\Gamma(A)$ always shares at least one common boundary point with $F(A)$, namely $\delta_1(A) + \mathrm{i}u(A)$. The shell of a square matrix can also be used to generate a spectral inclusion subset of the standard numerical range, the envelope, which is defined as $\mathcal{E}(A) = \bigcap_{\theta \in [0,2\pi]} e^{-\mathrm{i}\theta}\Gamma_{in}(e^{\mathrm{i}\theta}A)$. For more information on the envelope, see [3], [4], [14], [15] and the references therein.

Below, some properties of the shell are listed for reference. Let $A \in M_n(\mathbb{C})$, then

*Received by the editors on March 18, 2023. Accepted for publication on November 2, 2023. Handling Editor: Michael Tsatsomeros. Corresponding Author: Christos Chorianopoulos.

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Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 39, pp. 572-590, November 2023.

(S1) $\Gamma(V^*AV) = \Gamma(A)$, for any unitary matrix $V \in M_n(\mathbb{C})$.
(S2) $\Gamma(A + rI_n) = \Gamma(A) + r$, for all $r \in \mathbb{C}$.
(S3) If A is a real matrix, then $\Gamma(A)$ is symmetric with respect to the real axis.

As a comment on Property S2, note that

$$u(A + rI_n) = \mathrm{Im}\{\mathbf{y}_1^* K(A + rI_n)\mathbf{y}_1\} = u(A) + \mathrm{Im}\{r\}, \tag{1.3}$$

$$\nu(A + rI_n) = \|K(A + rI_n)\mathbf{y}_1\|_2^2 = \nu(A) + \mathrm{Im}\{r\}^2 + 2\,\mathrm{Im}\{r\}u(A). \tag{1.4}$$

Equations (1.3) and (1.4) yield one more property for the quantities $\nu(A), u(A)$, and $D(A)$, which will be used throughout the text.

(S4) $\nu(A + rI_n) - u(A + rI_n)^2 = \nu(A) - u(A)^2$ and $D(A + rI_n) = D(A)$, for all $r \in \mathbb{C}$.
(S5) If $A \in M_n(\mathbb{C})$ is normal matrix, then the quantity $\nu(A) - u(A)^2$ vanishes and the shell is reduced to the union of the straight line $\ell_2 = \{\delta_2(A) + \mathrm{i}t,\ t \in \mathbb{R}\}$ and the singleton $\{\delta_1(A) + \mathrm{i}u(A)\}$.

For more details on the shell, its properties, and its various forms, see [2], [6], [14], and [15].

An eigenvalue on the boundary of the convex hull of the spectrum of A is called an extremal eigenvalue. An eigenvalue with equal algebraic and geometric multiplicities that its corresponding eigenspace is orthogonal to the eigenspaces of all other eigenvalues is called normal. In [6], focus was given to the case where $D(A) > 0$ and several geometric aspects of the closed branch of the shell were studied and proposed as measures of non-normality of the extremal eigenvalues of a square matrix A that can be surrounded by closed branches of the shells $\Gamma(e^{\mathrm{i}\theta}A),\ \theta \in [0, 2\pi]$.

Definition 1.1. *Let $A \in M_n(\mathbb{C})$, and let λ_0 be an extremal eigenvalue.*

(i) If for some $\theta \in [0, 2\pi]$ it is $D(e^{\mathrm{i}\theta}A) > 0$ and λ_0 is surrounded by the closed branch of the curve $e^{-\mathrm{i}\theta}\Gamma(e^{\mathrm{i}\theta}A)$, then λ_0 is called a shell extremal eigenvalue of A.
(ii) $\mathcal{A}(\lambda_0) = \{\theta \in [0, 2\pi] : D(e^{\mathrm{i}\theta}A) > 0$ and λ_0 is surrounded by the closed branch of $e^{-\mathrm{i}\theta}\Gamma(e^{\mathrm{i}\theta}A)\}$.

Here, we list a series of properties of shell extremal eigenvalues and the closed branches of the shells that surround them [6].

(SE1) If λ_0 is a shell extremal eigenvalue of a matrix $A \in M_n(\mathbb{C})$, then $e^{\mathrm{i}\theta}\lambda_0$ is the rightmost eigenvalue of the matrix $e^{\mathrm{i}\theta}A$ for all $\theta \in \mathcal{A}(\lambda_0)$. Moreover, it is the unique eigenvalue that lies in the complex zone $\mathcal{Z} = \{z = x + \mathrm{i}y : \dfrac{\delta_1(e^{\mathrm{i}\theta}A) + \delta_2(e^{\mathrm{i}\theta}A) + \sqrt{D(e^{\mathrm{i}\theta}A)}}{2} \le x \le \delta_1(e^{\mathrm{i}\theta}A),\ y \in \mathbb{R},\ \theta \in \mathcal{A}(\lambda_0)\}$.
(SE2) Let $A \in M_n(\mathbb{C})$ with $D(A) > 0$ and let λ_0 be the shell extremal eigenvalue surrounded by the closed branch of $\Gamma(A)$. Then $\mathcal{A}(\lambda_0) \subset (3\pi/2, 0] \cup [0, \pi/2)$. If A is real and $D(A) > 0$ (resp. $D(-A) > 0$), then $\mathcal{A}(\lambda_0)$ is of the form $(2\pi - a, 2\pi] \cup [0, a)$ (resp. $(\pi - a, \pi + a)$), for some $a \in (0, \pi/2)$ where λ_0 is the simple eigenvalue surrounded by the closed branch of $\Gamma(A)$ (resp. $-\Gamma(-A)$).
(SE3) If $\lambda_1, \lambda_2, \cdots, \lambda_k$ are the shell extremal eigenvalues of $A \in M_n(\mathbb{C})$, then $\mathcal{A}(\lambda_i) \cap \mathcal{A}(\lambda_j) = \emptyset$, for $i \ne j$, $i, j = 1, \ldots, k$ and $\{\theta \in [0, 2\pi] : D(e^{\mathrm{i}\theta}A) > 0\} = \bigcup_{i=1}^{k} \mathcal{A}(\lambda_i)$.
(SE4) The radius of curvature of $\Gamma(e^{\mathrm{i}\theta}A)$ at $\delta_1(e^{\mathrm{i}\theta}A) + \mathrm{i}u(e^{\mathrm{i}\theta}A)$, $\theta \in [0, 2\pi]$ is

$$R_{\Gamma(e^{\mathrm{i}\theta}A)}(\delta_1(e^{\mathrm{i}\theta}A) + \mathrm{i}u(e^{\mathrm{i}\theta}A)) = \frac{\nu(e^{\mathrm{i}\theta}A) - u(e^{\mathrm{i}\theta}A)^2}{2\,(\delta_1(e^{\mathrm{i}\theta}A) - \delta_2(e^{\mathrm{i}\theta}A))}.$$

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Volume 39, pp. 572-590, November 2023.

(SE5) For $\theta \in [0, 2\pi]$ such that $D(e^{i\theta}A) > 0$, the maximum distance between two points on the boundary of the closed branch is

$$d_h(e^{i\theta}A) = \frac{\delta_1(e^{i\theta}A) - \delta_2(e^{i\theta}A) - \sqrt{D(e^{i\theta}A)}}{2}.$$

(SE6) λ_0 is a normal shell extremal eigenvalue of a matrix A if and only if the closed branches of the curves $e^{-i\theta}\Gamma(e^{i\theta}A)$ are reduced to singletons for all $\theta \in \mathcal{A}(\lambda_0)$.

In this work, we examine the shell and the existence of shell extremal eigenvalues of non-normal tridiagonal Toeplitz matrices $T_n(c, b, a) \in M_n(\mathbb{C})$ of the form

$$T_n(c,b,a) = \begin{bmatrix} a & b & 0 & \cdots & 0 \\ c & a & b & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & c & a & b \\ 0 & \cdots & 0 & c & a \end{bmatrix}, \ |bc| \neq 0,\ |b| \neq |c|,\ n \geq 2. \tag{1.5}$$

Throughout the text, we set $b = |b|e^{i\theta_b}$ and $c = |c|e^{i\theta_c}$, when needed. The eigenvalues, and right and left eigenvectors of $T_n(c, b, a)$ are

$$\lambda_k = a + 2\sqrt{bc}\cos\left(\frac{k\pi}{n+1}\right), k = 1, 2, \ldots, n, \ \text{ and} \tag{1.6}$$

$$\mathbf{x}_k = [x_{k,1}, x_{k,2}, \cdots, x_{k,n}]^T, \ \ x_{k,j} = \left(\frac{c}{b}\right)^{\frac{j}{2}} \sin\left(\frac{kj\pi}{n+1}\right), j = 1, 2, \ldots, n, \tag{1.7}$$

$$\mathbf{x}_{l,k} = [w_{k,1}, w_{k,2}, \cdots, w_{k,n}]^T, \ \ w_{k,j} = \left(\frac{\overline{b}}{\overline{c}}\right)^{\frac{j}{2}} \sin\left(\frac{kj\pi}{n+1}\right), j = 1, 2, \ldots, n, \tag{1.8}$$

respectively (see [3], [5], [13] and the references therein). The eigenvalues of $T_n(c, b, a)$ are collinear. The reason why we assume $|b| \neq |c|$ is because if $|b| = |c|$ then $T_n(c, b, a)$ is a normal matrix, which follows directly by requiring $T_n(c, b, a)T_n(c, b, a)^* = T_n(c, b, a)^*T_n(c, b, a)$. Then the shells $\Gamma(e^{i\theta}T_n(c, b, a))$ reduce to unions of straight lines and singletons as is described in property S5. This particular case is of no interest for the present work and it is mostly ignored unless stated otherwise.

The structure of the paper is as follows. In Section 2, a complete description of the shells of the matrices $e^{i\theta}T_n(c, b, a)$, $\theta \in [0, 2\pi]$ is given and closed formulas for their related quantities are obtained. In Section 3, necessary and sufficient conditions are given for the existence of shell extremal eigenvalues for $T_n(c, b, a)$ and the angular sets $\mathcal{A}(\lambda)$ are fully described. In Section 4, some shell related quantities that measure the non-normality of shell extremal eigenvalues are evaluated. It is shown that these quantities are also measures of non-normality for the entire matrix $T_n(c, b, a)$ and a comparison to other such measures is done. In Section 5, some numerical examples are presented to illustrate the results.

2. The shell of $e^{i\theta}T_n(c, b, a)$.

We begin by describing the shell of $e^{i\theta}T_n(c, b, a)$ in (1.5). To that end, for the sake of simplicity of calculations and in view of properties S2 and S4, in some proofs we consider the translation

$$e^{i\theta}T_n(c, b, 0) = e^{i\theta}(T_n(c, b, a) - aI_n), \ \ |bc| \neq 0,\ |b| \neq |c|. \tag{2.9}$$

The hermitian and skew-hermitian parts of $e^{i\theta}T_n(c, b, 0)$ are

$$H(e^{i\theta}T_n(c, b, 0)) = \frac{1}{2}T_n(\overline{p(\theta)}, p(\theta), 0), \ \ p(\theta) = e^{i\theta}b + e^{-i\theta}\overline{c}, \tag{2.10}$$

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A publication of the International Linear Algebra Society
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and

$$K(e^{\mathrm{i}\theta}T_n(c,b,0)) = \frac{1}{2}T_n(-\overline{q(\theta)}, q(\theta), 0), \quad q(\theta) = e^{\mathrm{i}\theta}b - e^{-\mathrm{i}\theta}\overline{c}, \tag{2.11}$$

respectively. The eigenvalues of $H(e^{\mathrm{i}\theta}T_n(c,b,0))$ are

$$\delta_k(e^{\mathrm{i}\theta}T_n(c,b,0)) = |p(\theta)|\cos\left(\frac{k\pi}{n+1}\right), \; k = 1,2,\cdots,n, \tag{2.12}$$

with a choice for a corresponding unit eigenvector for $\delta_k(e^{\mathrm{i}\theta}T_n(c,b,0))$ being

$$\mathbf{y}_k(\theta) = \sqrt{\frac{2}{n+1}}[y_{k,1}, y_{k,2}, \ldots, y_{k,n}]^T, \quad y_{k,j} = \alpha(\theta)^{\frac{j}{2}}\sin\left(\frac{kj\pi}{n+1}\right), j = 1,2,\cdots,n, \tag{2.13}$$

where

$$\alpha(\theta) = \frac{\overline{p(\theta)}}{p(\theta)}. \tag{2.14}$$

The formulas in equations (2.12), (2.13), and (2.14) can also be found in [3].

The assumption that $|b| \neq |c|$ ensures that $|p(\theta)| \neq 0$. First a lemma is presented that connects all the quantities $b, c, \alpha(\theta), p(\theta)$, and $q(\theta)$.

LEMMA 2.1. *For the quantities $p(\theta)$, $q(\theta)$, and $\alpha(\theta)$ in (2.10), (2.11), and (2.14), respectively, it is*

$$|q(\theta)|^2 - \mathrm{Im}\left\{q(\theta)\alpha(\theta)^{\frac{1}{2}}\right\}^2 = \frac{\left(|b|^2 - |c|^2\right)^2}{|p(\theta)|^2}, \quad \theta \in [0, 2\pi], \quad |b| \neq |c|.$$

Proof.

$$\begin{aligned}
|q(\theta)|^2 - \mathrm{Im}\left\{q(\theta)\alpha(\theta)^{\frac{1}{2}}\right\}^2 &= |q(\theta)|^2 + \frac{1}{4}\left(q(\theta)\alpha(\theta)^{\frac{1}{2}} - \overline{q(\theta)}\overline{\alpha(\theta)^{\frac{1}{2}}}\right)^2 \\
&= |q(\theta)|^2 + \frac{1}{4}\left(q(\theta)^2\alpha(\theta) + \overline{q(\theta)}^2\overline{\alpha(\theta)} - 2|q(\theta)|^2\right) \\
&= \frac{|q(\theta)|^2}{2} + \frac{1}{2}\mathrm{Re}\left\{q(\theta)^2\alpha(\theta)\right\},
\end{aligned}$$

which yields

$$|q(\theta)|^2 - \mathrm{Im}\left\{q(\theta)\alpha(\theta)^{\frac{1}{2}}\right\}^2 = \frac{1}{2|p(\theta)|^2}\left[|q(\theta)p(\theta)|^2 + \mathrm{Re}\left\{(q(\theta)\overline{p(\theta)})^2\right\}\right]. \tag{2.15}$$

Note that $|q(\theta)|^2 = (be^{\mathrm{i}\theta} - \overline{c}e^{-\mathrm{i}\theta})(\overline{b}e^{-\mathrm{i}\theta} - ce^{\mathrm{i}\theta}) = |b|^2 + |c|^2 - 2|bc|\cos(2\theta + \theta_b + \theta_c)$, and similarly $|p(\theta)|^2 = (be^{\mathrm{i}\theta} + \overline{c}e^{-\mathrm{i}\theta})(\overline{b}e^{-\mathrm{i}\theta} + ce^{\mathrm{i}\theta}) = |b|^2 + |c|^2 + 2|bc|\cos(2\theta + \theta_b + \theta_c)$, so that

$$|q(\theta)p(\theta)|^2 = (|b|^2 + |c|^2)^2 - 4|bc|^2\cos^2(2\theta + \theta_b + \theta_c). \tag{2.16}$$

The real part involved in (2.15) is

$$\mathrm{Re}\left\{(q(\theta)\overline{p(\theta)})^2\right\} = \mathrm{Re}\left\{\left((be^{\mathrm{i}\theta} - \overline{c}e^{-\mathrm{i}\theta})(\overline{b}e^{-\mathrm{i}\theta} + ce^{\mathrm{i}\theta})\right)^2\right\}$$

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$$
\begin{aligned}
&= \operatorname{Re}\left\{\left(|b|^2-|c|^2+|bc|e^{\mathrm{i}(2\theta+\theta_b+\theta_c)}-|bc|e^{-\mathrm{i}(2\theta+\theta_b+\theta_c)}\right)^2\right\}\\
&= \operatorname{Re}\left\{\left(|b|^2-|c|^2+2|bc|\mathrm{i}\sin(2\theta+\theta_b+\theta_c)\right)^2\right\}\\
&= \operatorname{Re}\left\{(|b|^2-|c|^2)^2-4|bc|^2\sin^2(2\theta+\theta_b+\theta_c)+4\mathrm{i}(|b|^2-|c|^2)|bc|\sin(2\theta+\theta_b+\theta_c)\right\},
\end{aligned}
$$

so that

$$
\operatorname{Re}\left\{(q(\theta)\overline{p(\theta)})^2\right\} = (|b|^2-|c|^2)^2-4|bc|^2\sin^2(2\theta+\theta_b+\theta_c). \tag{2.17}
$$

Substituting (2.16) and (2.17) in (2.15) yields the result. ☐

The following trigonometric identities will be used to find formulas for the quantities involved in the equations of the shells $\Gamma(e^{\mathrm{i}\theta}T_n(c,b,a)),\ \theta\in[0,2\pi]$.

LEMMA 2.2. *For any $n\in\mathbb{N}, n\geq 2$,*

(i) $\displaystyle\sum_{k=2}^{n-1}\left[\sin\left(\frac{(k-1)\pi}{n+1}\right)\sin\left(\frac{(k+1)\pi}{n+1}\right)\right]=\frac{1}{2}\left(n\cos\left(\frac{2\pi}{n+1}\right)+1\right).$

(ii) $\displaystyle\sum_{k=1}^{n-1}\left[\sin\left(\frac{k\pi}{n+1}\right)\sin\left(\frac{(k+1)\pi}{n+1}\right)\right]=\frac{n+1}{2}\cos\left(\frac{\pi}{n+1}\right).$

Proof. (i)

$$
\begin{aligned}
&\sum_{k=2}^{n-1}\left[\cos\left(\frac{(k-1)\pi}{n+1}\right)\cos\left(\frac{(k+1)\pi}{n+1}\right)\right]\\
&=\frac{1}{2}\sum_{k=2}^{n-1}\left[\cos\left(\frac{2\pi}{n+1}\right)-\cos\left(\frac{2k\pi}{n+1}\right)\right]\\
&=\frac{n-2}{2}\cos\left(\frac{2\pi}{n+1}\right)-\frac{1}{2}\sum_{k=2}^{n-1}\cos\left(\frac{2k\pi}{n+1}\right)\\
&=\frac{n-2}{2}\cos\left(\frac{2\pi}{n+1}\right)-\frac{1}{2}\left(-1-\cos\left(\frac{2\pi}{n+1}\right)-\cos\left(\frac{2n\pi}{n+1}\right)\right)\\
&=\frac{1}{2}\left[(n-2)\cos\left(\frac{2\pi}{n+1}\right)+1+2\cos\left(\frac{2\pi}{n+1}\right)\right]\\
&=\frac{1}{2}\left(n\cos\left(\frac{2\pi}{n+1}\right)+1\right).
\end{aligned}
$$

(ii)

$$
\begin{aligned}
&\sum_{k=1}^{n-1}\left[\sin\left(\frac{k\pi}{n+1}\right)\sin\left(\frac{(k+1)\pi}{n+1}\right)\right]\\
&=\sum_{k=1}^{n-1}\left[\sin\left(\frac{k\pi}{n+1}\right)\left(\sin\left(\frac{k\pi}{n+1}\right)\cos\left(\frac{\pi}{n+1}\right)+\sin\left(\frac{\pi}{n+1}\right)\cos\left(\frac{k\pi}{n+1}\right)\right)\right]\\
&=\cos\left(\frac{\pi}{n+1}\right)\sum_{k=1}^{n-1}\sin^2\left(\frac{k\pi}{n+1}\right)+\frac{1}{2}\sin\left(\frac{\pi}{n+1}\right)\sum_{k=1}^{n-1}\sin\left(\frac{2k\pi}{n+1}\right)
\end{aligned}
$$

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$$
\begin{aligned}
&= \cos\left(\frac{\pi}{n+1}\right)\left[\frac{n+1}{2} - \sin^2\left(\frac{n\pi}{n+1}\right)\right] + \frac{1}{2}\sin\left(\frac{\pi}{n+1}\right)\sin\left(\frac{2\pi}{n+1}\right)\\
&= \cos\left(\frac{\pi}{n+1}\right)\left[\frac{n+1}{2} - \sin^2\left(\frac{n\pi}{n+1}\right)\right] + \sin^2\left(\frac{\pi}{n+1}\right)\cos\left(\frac{\pi}{n+1}\right)\\
&= \frac{n+1}{2}\cos\left(\frac{\pi}{n+1}\right). \qquad \square
\end{aligned}
$$

PROPOSITION 2.3. *Let $T_n(c,b,a)$ and $T_n(c,b,0)$ be as in (1.5) and in (2.9), respectively. Then,*

(i) $\nu(e^{\mathrm{i}\theta}T_n(c,b,0)) = \dfrac{(n-1)|q(\theta)|^2}{n+1}\sin^2\left(\dfrac{\pi}{n+1}\right) + \dfrac{\operatorname{Im}\left\{q(\theta)\alpha(\theta)^{\frac{1}{2}}\right\}^2}{n+1}\left(n\cos\left(\dfrac{2\pi}{n+1}\right)+1\right)$,

(ii) $u(e^{\mathrm{i}\theta}T_n(c,b,0)) = \operatorname{Im}\left\{q(\theta)\alpha(\theta)^{\frac{1}{2}}\right\}\cos\left(\dfrac{\pi}{n+1}\right)$,

(iii) $\nu(e^{\mathrm{i}\theta}T_n(c,b,a)) - u(e^{\mathrm{i}\theta}T_n(c,b,a))^2 = \dfrac{n-1}{n+1}\sin^2\left(\dfrac{\pi}{n+1}\right)\dfrac{(|b|^2-|c|^2)^2}{|p(\theta)|^2}$.

Proof. Let

$$
\mathbf{w}(\theta) = K(e^{\mathrm{i}\theta}T_n(c,b,0))\mathbf{y}_1(\theta) = \frac{1}{2}T_n(-\overline{q(\theta)}, q(\theta), 0)\mathbf{y}_1(\theta)
$$

or,

$$
\mathbf{w}(\theta) = \frac{1}{2}\sqrt{\frac{2}{n+1}}\begin{bmatrix} 0 & q(\theta) & 0 & \cdots & 0\\ -\overline{q(\theta)} & 0 & q(\theta) & \cdots & 0\\ \vdots & \ddots & \ddots & \ddots & \vdots\\ 0 & \cdots & -\overline{q(\theta)} & 0 & q(\theta)\\ 0 & \cdots & 0 & -\overline{q(\theta)} & 0\end{bmatrix}\begin{bmatrix} \alpha(\theta)^{\frac{1}{2}}\sin\left(\frac{\pi}{n+1}\right)\\ \alpha(\theta)^{\frac{2}{2}}\sin\left(\frac{2\pi}{n+1}\right)\\ \vdots\\ \alpha(\theta)^{\frac{n-1}{2}}\sin\left(\frac{(n-1)\pi}{n+1}\right)\\ \alpha(\theta)^{\frac{n}{2}}\sin\left(\frac{n\pi}{n+1}\right)\end{bmatrix}
$$

or,

$$
\mathbf{w}(\theta) = \sqrt{\frac{1}{2(n+1)}}\begin{bmatrix} q(\theta)\alpha(\theta)\sin\left(\frac{2\pi}{n+1}\right)\\ -\overline{q(\theta)}\alpha(\theta)^{\frac{1}{2}}\sin\left(\frac{\pi}{n+1}\right) + q(\theta)\alpha(\theta)^{\frac{3}{2}}\sin\left(\frac{3\pi}{n+1}\right)\\ \vdots\\ -\overline{q(\theta)}\alpha(\theta)^{\frac{n-2}{2}}\sin\left(\frac{(n-2)\pi}{n+1}\right) + q(\theta)\alpha(\theta)^{\frac{n}{2}}\sin\left(\frac{n\pi}{n+1}\right)\\ -\overline{q(\theta)}\alpha(\theta)^{\frac{n-1}{2}}\sin\left(\frac{(n-1)\pi}{n+1}\right)\end{bmatrix}. \tag{2.18}
$$

(i) Since $|\alpha(\theta)|=1$, we have

$$
\begin{aligned}
\nu(e^{\mathrm{i}\theta}T_n(c,b,0)) &= \left\|K(e^{\mathrm{i}\theta}T_n(c,b,0))\right\|_2^2 = \left\|\frac{1}{2}T_n(-\overline{q(\theta)}, q(\theta), 0)\mathbf{y}_1(\theta)\right\|_2^2 = \|\mathbf{w}(\theta)\|_2^2\\
&= \frac{1}{2(n+1)}\left\{|q(\theta)|^2\sin^2\left(\frac{2\pi}{n+1}\right)\right.\\
&\quad + \sum_{k=2}^{n-1}\left|-\overline{q(\theta)}\alpha(\theta)^{\frac{k-1}{2}}\sin\left(\frac{(k-1)\pi}{n+1}\right) + q(\theta)\alpha(\theta)^{\frac{k+1}{2}}\sin\left(\frac{(k+1)\pi}{n+1}\right)\right|^2\\
&\quad \left. + |q(\theta)|^2\sin^2\left(\frac{(n-1)\pi}{n+1}\right)\right\}.
\end{aligned} \tag{2.19}
$$

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Let us simplify the quantities involving k:

$$\begin{aligned}
&\left|-\overline{q(\theta)}\alpha(\theta)^{\frac{k-1}{2}}\sin\left(\frac{(k-1)\pi}{n+1}\right)+q(\theta)\alpha(\theta)^{\frac{k+1}{2}}\sin\left(\frac{(k+1)\pi}{n+1}\right)\right|^2\\
&\quad=\left(-\overline{q(\theta)}\alpha(\theta)^{\frac{k-1}{2}}\sin\left(\frac{(k-1)\pi}{n+1}\right)+q(\theta)\alpha(\theta)^{\frac{k+1}{2}}\sin\left(\frac{(k+1)\pi}{n+1}\right)\right)\\
&\qquad\times\left(-q(\theta)\overline{\alpha(\theta)}^{\frac{k-1}{2}}\sin\left(\frac{(k-1)\pi}{n+1}\right)+\overline{q(\theta)}\,\overline{\alpha(\theta)}^{\frac{k+1}{2}}\sin\left(\frac{(k+1)\pi}{n+1}\right)\right)\\
&\quad=|q(\theta)|^2\left(\sin^2\left(\frac{(k-1)\pi}{n+1}\right)+\sin^2\left(\frac{(k+1)\pi}{n+1}\right)\right)\\
&\qquad-\left(q^2(\theta)\alpha(\theta)+\overline{q^2(\theta)\alpha(\theta)}\right)\sin\left(\frac{(k-1)\pi}{n+1}\right)\sin\left(\frac{(k+1)\pi}{n+1}\right).
\end{aligned}$$

By adding and subtracting $2|q(\theta)|^2\sin\left(\frac{(k-1)\pi}{n+1}\right)\sin\left(\frac{(k+1)\pi}{n+1}\right)$, the complex modulus becomes

$$\begin{aligned}
&\left|-\overline{q(\theta)}\alpha(\theta)^{\frac{k-1}{2}}\sin\left(\frac{(k-1)\pi}{n+1}\right)+q(\theta)\alpha(\theta)^{\frac{k+1}{2}}\sin\left(\frac{(k+1)\pi}{n+1}\right)\right|^2\\
&\quad=|q(\theta)|^2\left\{\sin^2\left(\frac{(k-1)\pi}{n+1}\right)+\sin^2\left(\frac{(k+1)\pi}{n+1}\right)-2\sin\left(\frac{(k-1)\pi}{n+1}\right)\sin\left(\frac{(k+1)\pi}{n+1}\right)\right\}\\
&\qquad-\left(q^2(\theta)\alpha(\theta)+\overline{q^2(\theta)\alpha(\theta)}-2|q(\theta)|^2\right)\sin\left(\frac{(k-1)\pi}{n+1}\right)\sin\left(\frac{(k+1)\pi}{n+1}\right)\\
&\quad=|q(\theta)|^2\left\{\sin^2\left(\frac{(k-1)\pi}{n+1}\right)+\sin^2\left(\frac{(k+1)\pi}{n+1}\right)-2\sin\left(\frac{(k-1)\pi}{n+1}\right)\sin\left(\frac{(k+1)\pi}{n+1}\right)\right\}\\
&\qquad-\left(2\mathrm{i}\,\mathrm{Im}\left\{q(\theta)\alpha(\theta)^{\frac{1}{2}}\right\}\right)^2\sin\left(\frac{(k-1)\pi}{n+1}\right)\sin\left(\frac{(k+1)\pi}{n+1}\right).
\end{aligned}$$

Keeping in mind that $\sin\left(\frac{(n-1)\pi}{n+1}\right)=\sin\left(\frac{2\pi}{n+1}\right)$, equation (2.11) becomes

$$\begin{aligned}
\nu(e^{\mathrm{i}\theta}T_n(c,b,0))=\frac{|q(\theta)|^2}{2(n+1)}\times&\left\{2\sin^2\left(\frac{2\pi}{n+1}\right)+\sum_{k=2}^{n-1}\left[\sin^2\left(\frac{(k-1)\pi}{n+1}\right)+\sin^2\left(\frac{(k+1)\pi}{n+1}\right)\right]\right.\\
&\left.-2\sum_{k=2}^{n-1}\sin\left(\frac{(k-1)\pi}{n+1}\right)\sin\left(\frac{(k+1)\pi}{n+1}\right)\right\}\\
&+2\frac{\mathrm{Im}\left\{q(\theta)\alpha(\theta)^{\frac{1}{2}}\right\}^2}{n+1}\sum_{k=2}^{n-1}\sin\left(\frac{(k+1)\pi}{n+1}\right)\sin\left(\frac{(k-1)\pi}{n+1}\right).
\end{aligned}$$

Now, with the use of the identity $\sum_{k=1}^{n}\sin^2\left(\frac{k\pi}{n+1}\right)=\frac{n+1}{2}$ observe that

$$\sum_{k=2}^{n-1}\left[\sin^2\left(\frac{(k+1)\pi}{n+1}\right)+\sin^2\left(\frac{(k-1)\pi}{n+1}\right)\right]=n+1-2\sin^2\left(\frac{\pi}{n+1}\right)-2\sin^2\left(\frac{2\pi}{n+1}\right),$$

Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 39, pp. 572-590, November 2023.

and with the use of item (i) of Lemma 2.2, we obtain

$$\begin{aligned}\nu(e^{\mathrm{i}\theta}T_n(c,b,0)) &= \frac{|q(\theta)|^2}{2(n+1)}\left\{n+1-2\sin^2\left(\frac{\pi}{n+1}\right)-n\cos\left(\frac{2\pi}{n+1}\right)-1\right\}\\ &\quad+\frac{\mathrm{Im}\left\{q(\theta)\alpha(\theta)^{\frac{1}{2}}\right\}^2}{n+1}\left(n\cos\left(\frac{2\pi}{n+1}\right)+1\right)\\ &=\frac{(n-1)|q(\theta)|^2}{n+1}\sin^2\left(\frac{\pi}{n+1}\right)+\frac{\mathrm{Im}\left\{q(\theta)\alpha(\theta)^{\frac{1}{2}}\right\}^2}{n+1}\left(n\cos\left(\frac{2\pi}{n+1}\right)+1\right),\end{aligned}$$

which completes item (i).

(ii)

$$u(e^{\mathrm{i}\theta}T_n(c,b,0)) = \frac{1}{2}\,\mathrm{Im}\left\{\mathbf{y}_1(\theta)^*T_n(-\overline{q(\theta)},q(\theta),0)\mathbf{y}_1(\theta)\right\},$$

or,

$$u(e^{\mathrm{i}\theta}T_n(c,b,0)) = \frac{1}{2}\,\mathrm{Im}\left\{\mathbf{y}_1(\theta)^*\mathbf{w}(\theta)\right\}.$$

With the use of equation (2.18), we have

$$\begin{aligned}&\frac{1}{2}\mathbf{y}_1(\theta)^*\mathbf{w}(\theta)\\ &=\frac{1}{n+1}\left[\overline{\alpha(\theta)^{\frac{1}{2}}}\sin\left(\frac{\pi}{n+1}\right),\overline{\alpha(\theta)}\sin\left(\frac{2\pi}{n+1}\right),\cdots,\overline{\alpha(\theta)^{\frac{n}{2}}}\sin\left(\frac{n\pi}{n+1}\right)\right]\\ &\quad\times\begin{bmatrix} q(\theta)\alpha(\theta)\sin\left(\frac{2\pi}{n+1}\right)\\ -\overline{q(\theta)}\alpha(\theta)^{\frac{1}{2}}\sin\left(\frac{\pi}{n+1}\right)+q(\theta)\alpha(\theta)^{\frac{3}{2}}\sin\left(\frac{3\pi}{n+1}\right)\\ \vdots\\ -\overline{q(\theta)}\alpha(\theta)^{\frac{n-2}{2}}\sin\left(\frac{(n-2)\pi}{n+1}\right)+q(\theta)\alpha(\theta)^{\frac{n}{2}}\sin\left(\frac{n\pi}{n+1}\right)\\ -\overline{q(\theta)}\alpha(\theta)^{\frac{n-1}{2}}\sin\left(\frac{(n-1)\pi}{n+1}\right)\end{bmatrix}\end{aligned}$$

$$\begin{aligned}&=\frac{1}{n+1}\left\{q(\theta)\alpha(\theta)^{\frac{1}{2}}\sin\left(\frac{\pi}{n+1}\right)\sin\left(\frac{2\pi}{n+1}\right)-\overline{q(\theta)}\,\overline{\alpha(\theta)^{\frac{1}{2}}}\sin\left(\frac{(n-1)\pi}{n+1}\right)\sin\left(\frac{n\pi}{n+1}\right)\right.\\ &\quad\left.+\,q(\theta)\alpha(\theta)^{\frac{1}{2}}\sum_{k=2}^{n-1}\sin\left(\frac{(k+1)\pi}{n+1}\right)\sin\left(\frac{k\pi}{n+1}\right)-\overline{q(\theta)}\,\overline{\alpha(\theta)^{\frac{1}{2}}}\sum_{k=2}^{n-1}\sin\left(\frac{k\pi}{n+1}\right)\sin\left(\frac{(k-1)\pi}{n+1}\right)\right\}\\ &=\frac{1}{n+1}\left(q(\theta)\alpha(\theta)^{\frac{1}{2}}-\overline{q(\theta)}\,\overline{\alpha(\theta)^{\frac{1}{2}}}\right)\sum_{k=1}^{n-1}\sin\left(\frac{(k+1)\pi}{n+1}\right)\sin\left(\frac{k\pi}{n+1}\right),\end{aligned}$$

which the use of item (ii) of Lemma 2.2 yields

$$\frac{1}{2}\mathbf{y}_1(\theta)^*\mathbf{w}(\theta)=\frac{q(\theta)\alpha(\theta)^{\frac{1}{2}}-\overline{q(\theta)}\,\overline{\alpha(\theta)^{\frac{1}{2}}}}{2}\cos\left(\frac{\pi}{n+1}\right),$$

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A publication of the International Linear Algebra Society
Volume 39, pp. 572-590, November 2023.

or

$$\frac{1}{2}\mathbf{y}_1(\theta)^*\mathbf{w}(\theta) = \mathrm{i}\,\mathrm{Im}\left\{q(\theta)\alpha(\theta)^{\frac{1}{2}}\right\}\cos\left(\frac{\pi}{n+1}\right),$$

which completes the proof of item (ii).

(iii)

$$\begin{aligned}\nu(e^{\mathrm{i}\theta}T_n(c,b,0)) - u(e^{\mathrm{i}\theta}T_n(c,b,0))^2 &= \nu(e^{\mathrm{i}\theta}T_n(c,b,0)) - \frac{n+1}{n+1}u(e^{\mathrm{i}\theta}T_n(c,b,0))^2 \\ = \frac{(n-1)|q(\theta)|^2}{n+1}\sin^2\left(\frac{\pi}{n+1}\right) &+ \frac{\mathrm{Im}\left\{q(\theta)\alpha(\theta)^{\frac{1}{2}}\right\}^2}{n+1}\left\{n\cos\left(\frac{2\pi}{n+1}\right)+1-(n+1)\cos^2\left(\frac{\pi}{n+1}\right)\right\} \\ = \frac{(n-1)|q(\theta)|^2}{n+1}\sin^2\left(\frac{\pi}{n+1}\right) &+ \frac{\mathrm{Im}\left\{q(\theta)\alpha(\theta)^{\frac{1}{2}}\right\}^2}{n+1}(1-n)\sin^2\left(\frac{\pi}{n+1}\right),\end{aligned}$$

and so

$$\nu(e^{\mathrm{i}\theta}T_n(c,b,0)) - u(e^{\mathrm{i}\theta}T_n(c,b,0))^2 = \frac{n-1}{n+1}\sin^2\left(\frac{\pi}{n+1}\right)\left(|q(\theta)|^2 - \mathrm{Im}\left\{q(\theta)\alpha(\theta)^{\frac{1}{2}}\right\}^2\right).$$

Applying Lemma 2.1 and property S4 completes the proof. ∎

For the remainder and for the sake of brevity, we assign

$$A(n) = \left(\cos\left(\frac{\pi}{n+1}\right) - \cos\left(\frac{2\pi}{n+1}\right)\right)^2, \tag{2.20}$$

and

$$B(n) = \frac{n-1}{n+1}\sin^2\left(\frac{\pi}{n+1}\right). \tag{2.21}$$

Corollary 2.4. *Let $T_n(c,b,a)$ be as in (1.5). Then,*

(i) $D(e^{\mathrm{i}\theta}T_n(c,b,a)) = |p(\theta)|^2A(n) - 4B(n)\dfrac{(|b|^2-|c|^2)^2}{|p(\theta)|^2}$.

(ii) If for some $\theta\in[0,2\pi]$ it is $D(e^{\mathrm{i}\theta}T_n(c,b,a))>0$, then

(a) $d_h(e^{\mathrm{i}\theta}T_n(c,b,a)) = \dfrac{\sqrt{|p(\theta)|^2A(n)} - \sqrt{|p(\theta)|^2A(n) - 4B(n)\dfrac{(|b|^2-|c|^2)^2}{|p(\theta)|^2}}}{2}$,

(b) $R_{\Gamma(e^{\mathrm{i}\theta}T_n(c,b,a))}(\delta_1(e^{\mathrm{i}\theta}T_n(c,b,a)) + \mathrm{i}u(e^{\mathrm{i}\theta}T_n(c,b,a))) = \dfrac{B(n)(|b|^2-|c|^2)^2}{2\sqrt{A(n)}|p(\theta)|^3}$.

Proof. With the use of equations (2.12) and (2.20), observe that

$$\begin{aligned}\delta_1(e^{\mathrm{i}\theta}T_n(c,b,a)) - \delta_2(e^{\mathrm{i}\theta}T_n(c,b,a)) &= |p(\theta)|\cos\left(\frac{\pi}{n+1}\right) + \mathrm{Re}\{a\} - |p(\theta)|\cos\left(\frac{2\pi}{n+1}\right) - \mathrm{Re}\{a\} \\ &= |p(\theta)|\sqrt{A(n)}.\end{aligned} \tag{2.22}$$

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A publication of the International Linear Algebra Society
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(i) With the use of Proposition 2.3 (iii)

$$\begin{aligned} D(e^{\mathrm{i}\theta}T_n(c,b,a)) &= \big(\delta_1(e^{\mathrm{i}\theta}T_n(c,b,a))\big) - \delta_2(e^{\mathrm{i}\theta}T_n(c,b,a)))^2 - 4\left(\nu(e^{\mathrm{i}\theta}T_n(c,b,a)) - u(e^{\mathrm{i}\theta}T_n(c,b,a))^2\right) \\ &= |p(\theta)|^2A(n) - 4\frac{n-1}{n+1}\sin^2\left(\frac{\pi}{n+1}\right)\frac{(|b|^2-|c|^2)^2}{|p(\theta)|^2}. \end{aligned}$$

Using (2.21), the result follows.

(ii) Item (ii,a) follows by combining property SE5, equation (2.22), and item (i). Item (ii,b) follows by property SE4, Proposition 2.3(iii), and equation (2.22). ◻

The shell of tridiagonal Toeplitz matrices satisfies certain symmetries. In [3], the authors in the process of showing that the envelope of the Toeplitz tridiagonal matrix in (1.5) is symmetric with respect to the point $a \in \mathbb{C}$ showed the following (see proof of Theorem 2.1 in [3]).

Proposition 2.5. *For the matrix $T_n(c,b,a)$ it is $\Gamma(e^{\mathrm{i}\theta}T_n(c,b,a)) = \Gamma(e^{\mathrm{i}(\pi+\theta)}T_n(c,b,a))$, for all $\theta \in [0,2\pi]$.*

3. Shell extremal eigenvalues. As is described in the introduction, the existence of shell extremal eigenvalues for a square matrix A depends on whether the function $D(e^{\mathrm{i}\theta}A)$, $\theta \in [0,2\pi]$ assumes positive values or not.

Proposition 3.1. *Let $T_n(c,b,a)$ be as in (1.5). Then, $D(e^{\mathrm{i}\theta}T_n(c,b,a)) > 0$ for some $\theta \in [0,2\pi]$ if and only if $\frac{||b|-|c||}{|b|+|c|}\sqrt{\frac{B(n)}{A(n)}} < \frac{1}{2}$.*

Proof. Recalling that $|p(\theta)|^2 = p(\theta)\overline{p(\theta)} = |b|^2+|c|^2+2|bc|\cos(2\theta+\theta_b+\theta_c)$ and assigning $\phi = 2\theta+\theta_b+\theta_c$, we have

$$\begin{aligned} D(e^{\mathrm{i}\theta}T_n(c,b,a)) > 0 &\Leftrightarrow \\ |p(\theta)|^2A(n) - 4B(n)\frac{(|b|^2-|c|^2)^2}{|p(\theta)|^2} > 0 &\Leftrightarrow \\ |p(\theta)|^4A(n) - 4B(n)(|b|^2-|c|^2)^2 > 0 &\Leftrightarrow \\ (|b|^2+|c|^2+2|bc|\cos(\phi))^2A(n) - 4B(n)(|b|^2-|c|^2)^2 > 0 & \end{aligned}$$

which yields

$$4|bc|^2A(n)\cos^2(\phi) + 4|bc|(|b|^2+|c|^2)A(n)\cos(\phi) + A(n)(|b|^2+|c|^2)^2 - 4B(n)(|b|^2-|c|^2)^2 > 0. \tag{3.23}$$

The quadratic polynomial in (3.23) is in $\cos(\phi)$. Its discriminant is

$$\begin{aligned} \Delta &= 16|bc|^2(|b|^2+|c|^2)^2A(n)^2 - 16|bc|^2A(n)\left[A(n)(|b|^2+|c|^2)^2 - 4B(n)(|b|^2-|c|^2)^2\right] \\ &= 16|bc|^2A(n)\left[(|b|^2+|c|^2)^2A(n) - A(n)(|b|^2+|c|^2)^2 + 4B(n)(|b|^2-|c|^2)^2\right] \\ &= 64|bc|^2(|b|^2-|c|^2)^2A(n)B(n) > 0, \end{aligned}$$

and its two distinct roots are

$$r_1 = -\frac{|b|^2+|c|^2}{2|bc|} - \frac{\left||b|^2-|c|^2\right|}{|bc|}\sqrt{\frac{B(n)}{A(n)}},$$

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A publication of the International Linear Algebra Society
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and

$$r_2 = -\frac{|b|^2+|c|^2}{2|bc|} + \frac{\big||b|^2-|c|^2\big|}{|bc|}\sqrt{\frac{B(n)}{A(n)}}.$$

Therefore, the quadratic attains positive values for some ϕ when $[-1,1]$ is not a subset of $[r_1,r_2], r_1<r_2$. Since $|bc|\neq 0$ and $|b|\neq|c|$, it is $(|b|-|c|)^2>0 \Rightarrow |b|^2+|c|^2>2|bc| \Rightarrow -\dfrac{|b|^2+|c|^2}{2|bc|}<-1$ which then yields that $r_1<-1$. As $r_1<-1$, the quadratic is positive for some ϕ (and so does $D(e^{\mathrm{i}\theta}T_n(c,b,a))$) if and only if $r_2<1$. That is because if $r_2<1$ then, as $\phi=2\theta+\theta_b+\theta_c,\ \theta\in[0,2\pi]$, there is some ϕ such that $r_2<\cos(\phi)<1$. Thus,

$$\begin{aligned}
&r_2<1\\
&\quad\Leftrightarrow -\frac{|b|^2+|c|^2}{2|bc|} + \frac{\big||b|^2-|c|^2\big|}{|bc|}\sqrt{\frac{B(n)}{A(n)}}<1\\
&\quad\Leftrightarrow \frac{\big||b|^2-|c|^2\big|}{|bc|}\sqrt{\frac{B(n)}{A(n)}}<\frac{|b|^2+|c|^2}{2|bc|}+1\\
&\quad\Leftrightarrow \frac{\big||b|^2-|c|^2\big|}{|bc|}\sqrt{\frac{B(n)}{A(n)}}<\frac{(|b|+|c|)^2}{2|bc|}\\
&\quad\Leftrightarrow \frac{||b|-|c||}{|b|+|c|}\sqrt{\frac{B(n)}{A(n)}}<\frac{1}{2},
\end{aligned}$$

which completes the proof. □

All eigenvalues of $T_n(c,b,a)$ are extremal eigenvalues since they are collinear. Combining this with property SE1 leads to the obvious conclusion that $T_n(c,b,a)$ can have at most two shell extremal eigenvalues, namely $\lambda_1=a+2\sqrt{bc}\cos(\frac{\pi}{n+1})$ and $\lambda_n=a+2\sqrt{bc}\cos(\frac{n\pi}{n+1})$. Proposition 2.5 ensures that if λ_1 is a shell extremal eigenvalue the same will be true for λ_n, and conversely. Therefore, with the use of Proposition 3.1, the next result is evident.

PROPOSITION 3.2. *$T_n(c,b,a)$ as in (1.5) has either none or two shell extremal eigenvalues. The latter occurs if and only if* $\dfrac{||b|-|c||}{|b|+|c|}\sqrt{\dfrac{B(n)}{A(n)}}<\dfrac{1}{2}$.

COROLLARY 3.3. *Let $T_n(c,b,a)$ as in (1.5) have two shell extremal eigenvalues, that is,* $\dfrac{||b|-|c||}{|b|+|c|}\sqrt{\dfrac{B(n)}{A(n)}}<\dfrac{1}{2}$. *Then every principal submatrix of the form $T_m(c,b,a),\ 2\le m<n$ obtained by deleting the last $n-m$ rows and columns of $T_n(c,b,a)$ also has shell extremal eigenvalues.*

Proof. By Proposition 3.2, it suffices to show that the sequence $\sqrt{\dfrac{B(k)}{A(k)}},\ k\ge 2$, is increasing.

$$\sqrt{\frac{B(k)}{A(k)}}=\sqrt{\frac{k-1}{k+1}}\cdot\frac{\sin\left(\dfrac{\pi}{k+1}\right)}{\cos\left(\dfrac{\pi}{k+1}\right)-\cos\left(\dfrac{2\pi}{k+1}\right)}$$

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A publication of the International Linear Algebra Society
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$$= \sqrt{\frac{k-1}{k+1}} \cdot \frac{2\sin\left(\frac{\pi}{2(k+1)}\right)\cos\left(\frac{\pi}{2(k+1)}\right)}{2\sin\left(\frac{\pi}{2(k+1)}\right)\sin\left(\frac{3\pi}{2(k+1)}\right)}$$
$$= \sqrt{\frac{k-1}{k+1}} \cdot \frac{\cos\left(\frac{\pi}{2(k+1)}\right)}{\sin\left(\frac{3\pi}{2(k+1)}\right)},$$

which is the product of two positive increasing sequences, and the proof is complete. ∎

Remark 3.4. *By Corollary 2.4, we can see that the function $D(e^{\mathrm{i}\theta}T_n(c,b,a))$, $\theta \in [0,2\pi]$ attains its maximum where $|p(\theta)|$ also does. Recall that $|p(\theta)|^2 = |b|^2 + |c|^2 + 2|bc|\cos(2\theta + \theta_b + \theta_c)$ which attains its maximum at $\phi_1 = -\frac{\theta_b+\theta_c}{2}$ and $\phi_2 = \pi - \frac{\theta_b+\theta_c}{2}$, and $|p(\phi_i)|^2 = (|b|+|c|)^2$, $i = 1, 2$.*

Slightly altering a technique in [9], the next lemma reveals something interesting about the rotations ϕ_1 and ϕ_2 of $T_n(c,b,0)$.

Lemma 3.5. *$T_n(c,b,0)$ in (2.9) is rotationally unitarily similar to a real matrix.*

Proof. We will show that for the matrix $e^{-\mathrm{i}\frac{\theta_b+\theta_c}{2}}T_n(c,b,0) = T_n(\hat{c},\hat{b},0)$, $\hat{b} = |b|e^{\mathrm{i}\frac{\theta_b-\theta_c}{2}}$, $\hat{c} = |c|e^{-\mathrm{i}\frac{\theta_b-\theta_c}{2}}$, there is a unitary transformation that turns it into a real tridiagonal matrix. Consider the unitary diagonal matrix U with diagonal entries $u_i = e^{\mathrm{i}(i-2)\frac{\theta_b-\theta_c}{2}}$, $i = 1, 2, \cdots, n$. Then,

$$UT_n(\hat{c},\hat{b},0)U^* = \begin{bmatrix} u_1 & & & & \\ & u_2 & & & \\ & & \ddots & & \\ & & & u_{n-1} & \\ & & & & u_n \end{bmatrix} \begin{bmatrix} 0 & \hat{b} & & & \\ \hat{c} & 0 & \hat{b} & & \\ & \ddots & \ddots & \ddots & \\ & & \hat{c} & 0 & \hat{b} \\ & & & \hat{c} & 0 \end{bmatrix} \begin{bmatrix} \overline{u_1} & & & & \\ & \overline{u_2} & & & \\ & & \ddots & & \\ & & & \overline{u_{n-1}} & \\ & & & & \overline{u_n} \end{bmatrix}$$
$$= \begin{bmatrix} 0 & u_1\overline{u_2}\hat{b} & & & \\ \overline{u_1}u_2\hat{c} & 0 & u_2\overline{u_3}\hat{b} & & \\ & \ddots & \ddots & \ddots & \\ & & \overline{u_{n-2}}u_{n-1}\hat{c} & 0 & u_{n-1}\overline{u_n}\hat{b} \\ & & & \overline{u_{n-1}}u_n\hat{c} & 0 \end{bmatrix}.$$

The nonzero entries of UAU^* are

$$u_i\overline{u_{i+1}}\hat{b} = |b|e^{\mathrm{i}(i-2-i+1+1)\frac{\theta_b-\theta_c}{2}} = |b| \in \mathbb{R},\ i = 1, \cdots, n,$$

and

$$\overline{u_i}u_{i+1}\hat{c} = |c|e^{\mathrm{i}(-i+2+i-1-1)\frac{\theta_b-\theta_c}{2}} = |c| \in \mathbb{R},\ i = 1, \cdots, n,$$

which completes the proof. ∎

Next, a complete characterization of the angular sets $\mathcal{A}(\lambda_k)$, $k = 1, n$ of Definition 1.1 is given.

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A publication of the International Linear Algebra Society
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Proposition 3.6. *Let $T_n(c,b,a)$ as in (1.5) be such that* $\frac{||b|-|c||}{|b|+|c|}\sqrt{\frac{B(n)}{A(n)}}<\frac{1}{2}$ *and let* $r_2=-\frac{|b|^2+|c|^2}{2|bc|}+\frac{\left||b|^2-|c|^2\right|}{|bc|}\sqrt{\frac{B(n)}{A(n)}}$. *Then, the angular sets $\mathcal{A}(\lambda_k),\ k=1,n$ are determined by*

$$\theta_1=\left(-\frac{\arccos(r_2)}{2}-\frac{\theta_b+\theta_c}{2}\right)\bmod 2\pi,\ \ \theta_2=\left(\frac{\arccos(r_2)}{2}-\frac{\theta_b+\theta_c}{2}\right)\bmod 2\pi,$$

$$\theta_3=(\pi+\theta_1)\bmod 2\pi,\ \ \theta_4=(\pi+\theta_2)\bmod 2\pi,$$

and they can be of the following forms:

$$(\theta_1,\theta_2)\ \text{ or }\ (\theta_1,2\pi)\cup[0,\theta_2),\ \text{ and }\ (\theta_3,\theta_4)\ \text{ or }\ (\theta_3,2\pi)\cup[0,\theta_4).$$

Proof. In view of property S2 in the introduction, without loss of generality we can work with $T_n(c,b,0)$. According to Proposition 3.2, the assumption that $\frac{||b|-|c||}{|b|+|c|}\sqrt{\frac{B(n)}{A(n)}}<\frac{1}{2}$ ensures the existence of shell extremal eigenvalues, and therefore, the non-emptiness of $\mathcal{A}(\lambda_k),\ k=1,n$. By Definition 1.1, property SE3 and the fact that $T_n(c,b,0)$ has two shell extremal eigenvalues, namely $\lambda_1=2\sqrt{bc}\cos\left(\frac{\pi}{n+1}\right)=-\lambda_n$, it is $\mathcal{A}(\lambda_1)\cup\mathcal{A}(\lambda_n)=\{\theta\in[0,2\pi]:D(e^{\mathrm{i}\theta}T_n(c,b,0))>0\}$. Moreover, observe that by Corollary 2.4 $D(e^{\mathrm{i}\theta}T_n(c,b,0))$ is continuous in θ. Thus, the angular sets $\mathcal{A}(\lambda_k)\subset[0,2\pi],\ k=1,n$, are either connected or they are the union of intervals (the latter is because we demand the sets $\mathcal{A}(\lambda_k)$ to be a subsets of $[0,2\pi]$).

Observe that,

$$D(e^{\mathrm{i}\theta}T_n(c,b,0))=D\left(e^{\mathrm{i}\left(\theta+\frac{\theta_b+\theta_c}{2}\right)}e^{-\mathrm{i}\frac{\theta_b+\theta_c}{2}}T_n(c,b,0)\right)=D\left(e^{\mathrm{i}\left(\theta+\frac{\theta_b+\theta_c}{2}\right)}T_n(\hat{c},\hat{b},0)\right)=D(e^{\mathrm{i}\hat{\theta}}T_n(\hat{c},\hat{b},0)),$$

where $\hat{\theta}=\theta+\frac{\theta_b+\theta_c}{2}$, $\hat{b}=|b|e^{\mathrm{i}\frac{\theta_b-\theta_c}{2}}$ and $\hat{c}=|c|e^{-\mathrm{i}\frac{\theta_b-\theta_c}{2}}$. The condition of Proposition 3.2 is still satisfied and since $T_n(\hat{c},\hat{b},0)$ is unitarily similar to a real matrix with $D(\pm T_n(\hat{c},\hat{b},0))>0$, properties SE2, SE3 and Proposition 2.5 yield $\mathcal{A}(\hat{\lambda}_1)=(2\pi-a,2\pi]\cup[0,a)$, $\mathcal{A}(\hat{\lambda}_n)=(\pi-a,\pi+a)=\{\pi+r:r\in\mathcal{A}(\hat{\lambda}_1)\}$, for some $a\in(0,\pi/2)$ and $\mathcal{A}(\hat{\lambda}_1)\cup\mathcal{A}(\hat{\lambda}_2)=\{\hat{\theta}\in[0,2\pi]:D(e^{\mathrm{i}\hat{\theta}}T_n(\hat{c},\hat{b},0))>0\}$, where $\hat{\lambda}_k,\ k=1,n$ are the two shell extremal eigenvalues of $T_n(\hat{c},\hat{b},0)$. As was seen in the proof of Proposition 3.1, $D(e^{\mathrm{i}\hat{\theta}}T_n(\hat{c},\hat{b},0))>0$ if and only if $\cos(2\hat{\theta}+\theta_{\hat{b}}+\theta_{\hat{c}})>r_2$, therefore $D(e^{\mathrm{i}\theta}T_n(c,b,0))=D(e^{\mathrm{i}\hat{\theta}}T_n(\hat{c},\hat{b},0))>0$ if and only if $r_2<\cos(2\hat{\theta}+\theta_{\hat{b}}+\theta_{\hat{c}})$, and observing that $\theta_{\hat{b}}+\theta_{\hat{c}}=0$, we have

$$-\arccos(r_2)<2\hat{\theta}<\arccos(r_2)\Leftrightarrow-\frac{\arccos(r_2)}{2}<\hat{\theta}<\frac{\arccos(r_2)}{2}.$$

Without loss of generality, we consider $\arccos(r_2)\in(0,\pi)\Rightarrow a=\frac{\arccos(r_2)}{2}\in(0,\pi/2)$. Recalling that $\hat{\theta}=\theta+\frac{\theta_b+\theta_c}{2}$, we can conclude that one of the sets $\mathcal{A}(\lambda_k),\ k=1,n$ is of one of the forms (θ_1,θ_2) or $(\theta_1,2\pi)\cup[0,\theta_2)$ and the other one is of the form (θ_3,θ_4) or $(\theta_3,2\pi)\cup[0,\theta_4)$. ∎

We conclude this section with some remarks on the envelope $\mathcal{E}(T_n(c,b,a))$ related to what has preceded. The envelope of a square matrix A gives a better spectral approximation in comparison to the standard numerical range, but it is not in general connected. Moreover, sufficient conditions for the connectedness of

Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 39, pp. 572-590, November 2023.

the envelope and lower or upper bounds for the number of its connected components are yet to arise in the literature. However, for the 2-rank numerical range [7, 8, 12, 16] defined as

$$F_2(A) = \bigcap_{\theta\in[0,2\pi]} \{e^{-\mathrm{i}\theta}(x+\mathrm{i}y) : x, y \in \mathbb{R},\ x \le \delta_2(e^{\mathrm{i}\theta}A)\},$$

it holds $F_2(A) \subseteq \mathcal{E}(A)$ (Theorem 3.1 of [15]).

Proposition 3.7. *Let $T_n(c,b,a)$ be as in (1.5), $n \ge 3$.*

(i) The eigenvalues $\lambda_k,\ k = 2,\cdots,n-1$ belong to a single connected component of $\mathcal{E}(T_n(c,b,a))$.

(ii) If $\frac{||b|-|c||}{|b|+|c|}\sqrt{\frac{B(n)}{A(n)}} < \frac{1}{2}$, then $\mathcal{E}(T_n(c,b,a))$ is disconnected. Especially, 3 is a lower bound for the number of its connected components.

Proof. (i) For $n = 3$, the result is evident. For $n \ge 4$ in view of properties P2, P3, and P4 in [15] and Lemma 3.5, without loss of generality we can work with the matrix $T_n(c,b,0),\ c > 0, b > 0$. Also in view of property (i) of Section 2 in [8] and Theorem 3.1 of [15] it suffices to show that the real eigenvalues $\lambda_k = 2\sqrt{bc}\cos\left(\frac{k\pi}{n+1}\right) \in F_2(T_n(c,b,0))$, $k = 2,3,\cdots,n-1$. $F_2(T_n(c,b,0))$ is an elliptical disc with major length $L = \sqrt{2\left(1+\cos\left(\frac{4\pi}{n+1}\right)\right)}(b+c)$ and foci the eigenvalues λ_2 and $\lambda_{n-1} = -\lambda_2$ (Theorem 12 and Proposition 13 of [1]). Thus, the convexity of $F_2(T_n(c,b,a))$ yields that the line segment created by these two eigenvalues, and which contains $\lambda_3,\lambda_4,\cdots,\lambda_{n-2}$, is contained if $F_2(T_n(c,b,a))$, which proves item (i).

(ii) A sufficient condition for $\mathcal{E}(T_n(c,b,a))$ to be disconnected is, of course, $\frac{||b|-|c||}{|b|+|c|}\sqrt{\frac{B(n)}{A(n)}} < \frac{1}{2}$. Then for some θ_0, in view of Propositions 3.1 and 2.5, the shells $\Gamma(e^{\mathrm{i}\theta_0}T_n(c,b,a))$ and $\Gamma(e^{\mathrm{i}(\pi+\theta_0)}T_n(c,b,a))$ are not connected, forcing the envelope to be as such. Both these shells form closed branches that contain one of each shell extremal eigenvalue. Item (i) completes the proof. ∎

4. Measures of non-normality.

4. Measures of non-normality. Motivated by property SE6 in the introduction, the following quantities can be considered as measures of non-normality of a shell extremal eigenvalue λ_0 of $A \in M_n(\mathbb{C})$ as they vanish if and only if λ_0 is a normal eigenvalue [6].

- $\eta_{1,A}(\lambda_0) = \inf\left\{d_h\left(e^{\mathrm{i}\theta}A\right) : \theta \in \mathcal{A}(\lambda_0)\right\}$,
- $\eta_{2,A}(\lambda_0) = \inf\left\{\nu\left(e^{\mathrm{i}\theta}A\right) - u\left(e^{\mathrm{i}\theta}A\right)^2 : \theta \in \mathcal{A}(\lambda_0)\right\}$,
- $\eta_{3,A}(\lambda_0) = \inf\left\{R_{\Gamma(e^{\mathrm{i}\theta}A)}(\delta_1(e^{\mathrm{i}\theta}A) + \mathrm{i}u(e^{\mathrm{i}\theta}A)) : \theta \in \mathcal{A}(\lambda_0)\right\}$.

The next proposition gives explicit expressions for the measures of non-normality of shell extremal eigenvalues $n_{i,T_n(c,b,a)}(\cdot),\ i = 1,2,3$.

Proposition 4.1. *Let $T_n(c,b,a)$ in equation (1.5), be such that $\frac{||b|-|c||}{|b|+|c|}\sqrt{\frac{B(n)}{A(n)}} < \frac{1}{2}$. Let also $\lambda_k,\ k = 1,n$ be the two shell extremal eigenvalues. Then,*

(i) $n_{1,T_n(c,b,a)}(\lambda_k) = \frac{1}{2}\left(\sqrt{(|b|+|c|)^2A(n)} - \sqrt{(|b|+|c|)^2A(n) - 4B(n)(|b|-|c|)^2}\right),\ k = 1,n,$

(ii) $n_{2,T_n(c,b,a)}(\lambda_k) = B(n)(|b|-|c|)^2,\ k = 1,n,$

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A publication of the International Linear Algebra Society
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(iii) $n_{3,T_n(c,b,a)}(\lambda_k) = \dfrac{B(n)(|b|-|c|)^2}{2\sqrt{A(n)}(|b|+|c|)}$, $k = 1, n$.

Moreover, the infima are obtained at the same points for λ_1 and λ_n, respectively.

Proof. As is described in Remark 3.4, $|p(\theta)|$, $\theta \in [0, 2\pi]$, attains its maximum at $\phi_1 = -\frac{\theta_b+\theta_c}{2}$ and $\phi_2 = \pi - \frac{\theta_b+\theta_c}{2}$, and $|p(\phi_1)|^2 = |p(\phi_2)|^2 = (|b|+|c|)^2$. By Propositions 2.3 (iii) and Corollary 2.4, it is evident that both $\nu(e^{i\theta}T_n(c,b,a)) - u(e^{i\theta}T_n(c,b,a))^2$ and $R_{\Gamma(e^{i\theta}T_n(c,b,a))}(\delta_1(e^{i\theta}T_n(c,b,a)) + iu(e^{i\theta}T_n(c,b,a)))$ are minimized where $|p(\theta)|$ is maximum. Thus,

$$n_{2,T_n(c,b,a)}(\lambda_k) = B(n)(|b|-|c|)^2, \quad k = 1, n,$$

and

$$n_{3,T_n(c,b,a)}(\lambda_k) = \frac{B(n)(|b|-|c|)^2}{\sqrt{A(n)}(|b|+|c|)}, \quad k = 1, n.$$

Finally, observe that

$$d_h(e^{i\theta}T_n(c,b,a)) = \frac{\sqrt{|p(\theta)|^2 A(n)} - \sqrt{|p(\theta)|^2 A(n) - 4B(n)\dfrac{(|b|^2-|c|^2)^2}{|p(\theta)|^2}}}{2}$$

or,

$$d_h(e^{i\theta}T_n(c,b,a)) = \frac{2B(n)\dfrac{(|b|^2-|c|^2)^2}{|p(\theta)|^2}}{\sqrt{|p(\theta)|^2 A(n)} + \sqrt{|p(\theta)|^2 A(n) - 4B(n)\dfrac{(|b|^2-|c|^2)^2}{|p(\theta)|^2}}},$$

and $d_h(e^{i\theta}T_n(c,b,a))$ is minimized where $|p(\theta)|$ is maximum. Substituting $|p(\phi_1)|^2 = |p(\phi_2)|^2 = (|b|+|c|)^2$ into item (iia) of Corollary 2.4 yields the result for $n_{1,T_n(c,b,a)}(\lambda_k)$. ☐

As was previously discussed, a tridiagonal Toeplitz matrix $T_n(c,b,a)$ is normal if and only if $|b| = |c|$. It is only natural to expect that measures of non-normality of such matrices will vanish if and only if $|b|-|c| = 0$. In [13], it was shown that the (Henrici) departure from normality [10] is equal to

$$\Delta_F(T_n(c,b,a)) = \sqrt{n-1}\,||b|-|c||\,, \tag{4.24}$$

and the structured distance from normality is equal to

$$\delta_F(T_n(c,b,a), \mathcal{N}_T) = \sqrt{\frac{n-1}{2}}\,||b|-|c||\,, \tag{4.25}$$

where both are considered with respect to the Frobenius norm (hence the index F in both Δ_F and δ_F). In equation (4.25) $\mathcal{N}_T$ denotes not the set of normal matrices of $M_n(\mathbb{C})$, but the set of normal complex tridiagonal Toeplitz matrices. Observe that the difference $|b|-|c|$ appears also in all the quantities $n_{i,T_n(c,b,a)}(\cdot)$. The next proposition illustrates why this is so.

Proposition 4.2. *The matrix $T_n(c,b,a)$ in equation (1.5) (but with the condition $|b| \neq |c|$ relaxed) is normal if and only if it has one normal eigenvalue.*

Proof. If $T_n(c,b,a)$ is normal, then the normality of all eigenvalues follows. For the converse, let $\lambda_k = a + 2\sqrt{bc}\cos\left(\dfrac{k\pi}{n+1}\right)$ for some $k \in \{1, 2, ..., n\}$ be a normal eigenvalue of $T_n(c,b,a)$. Then, its one-dimensional

Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 39, pp. 572-590, November 2023.

right eigenspace coincides with its left eigenspace. The right and left eigenvectors $\mathbf{x}_k$ and $\mathbf{x}_{l,k}$ of $T_n(c,b,a)$ for λ_k are given in (1.7) and (1.8), respectively. So there must be a nonzero $m \in \mathbb{C}$ such that

$$\mathbf{x}_k = m\mathbf{x}_{l,k}.$$

As,

$$\mathbf{x}_k = \left[\left(\frac{c}{b}\right)^{\frac{1}{2}} \sin\left(\frac{k\pi}{n+1}\right), \left(\frac{c}{b}\right)^{\frac{2}{2}} \sin\left(\frac{2k\pi}{n+1}\right), \cdots, \left(\frac{c}{b}\right)^{\frac{n}{2}} \sin\left(\frac{nk\pi}{n+1}\right)\right]^T,$$

and

$$\mathbf{x}_{l,k} = \left[\left(\frac{\bar{b}}{\bar{c}}\right)^{\frac{1}{2}} \sin\left(\frac{k\pi}{n+1}\right), \left(\frac{\bar{b}}{\bar{c}}\right)^{\frac{2}{2}} \sin\left(\frac{2k\pi}{n+1}\right), \cdots, \left(\frac{\bar{b}}{\bar{c}}\right)^{\frac{n}{2}} \sin\left(\frac{nk\pi}{n+1}\right)\right]^T,$$

it must be

$$\left(\frac{c}{b}\right)^{\frac{j}{2}} \sin\left(\frac{jk\pi}{n+1}\right) = m\left(\frac{\bar{b}}{\bar{c}}\right)^{\frac{j}{2}} \sin\left(\frac{jk\pi}{n+1}\right), \;\; j = 1, \cdots, n,$$

or

$$\left(\frac{|c|}{|b|}\right)^j = m, \;\; j = 1, \cdots, n.$$

The last condition must hold for all $j = 1, \cdots, n$, which clearly yields $m = 1$ and $|b| = |c|$, that is, $T_n(c,b,a)$ is a normal matrix. □

As a consequence of Proposition 4.2, we can conclude that measures of non-normality of an eigenvalue of $T_n(c,b,a)$ are actually measures of non-normality for the entire matrix. Thus, in the case where $T_n(c,b,a)$ has shell extremal eigenvalues and with the use of a continuity argument of $n_{i,T_n(c,b,a)}$ with respect to b and c the following result follows readily.

Corollary 4.3. *Let $T_n(c,b,a)$ be as in equation (1.5) (but with the condition $|b| \neq |c|$ relaxed) such that $\frac{||b|-|c||}{|b|+|c|}\sqrt{\frac{B(n)}{A(n)}} < \frac{1}{2}$. Then $T_n(c,b,a)$ is normal if and only if $n_{i,T_n(c,b,a)}(\lambda_k) = 0,\; i = 1,2,3,\; k = 1,n$.*

Corollary 4.4. *Let $T_n(c,b,a)$ in equation (1.5), be such that $\frac{||b|-|c||}{|b|+|c|}\sqrt{\frac{B(n)}{A(n)}} < \frac{1}{2}$. Let also $\lambda_k,\; k = 1,n$ be the two shell extremal eigenvalues. Then,*

(i) $n_{1,T_n(c,b,a)}(\lambda_k) \leq 4\delta_F(T_n(c,b,a)) \leq 4\Delta_F(T_n(c,b,a))$.
(ii) $\sqrt{n_{2,T_n(c,b,a)}(\lambda_k)} \leq \delta_F(T_n(c,b,a)) \leq \Delta_F(T_n(c,b,a))$.
(iii) $n_{3,T_n(c,b,a)}(\lambda_k) \leq \delta_F(T_n(c,b,a)) \leq \Delta_F(T_n(c,b,a))$.

Proof. By Corollary 3.14 of [6] we have that $n_{1,T_n(c,b,a)}(\lambda_k) \leq 4n_{3,T_n(c,b,a)}(\lambda_k)$. Moreover,

$$\begin{aligned}
n_{3,T_n(c,b,a)}(\lambda_k) &= \frac{B(n)(|b|-|c|)^2}{\sqrt{A(n)}||b|+|c||} < \frac{B(n)\,||b|-|c||}{\sqrt{A(n)}} = \frac{n-1}{n+1}\frac{\sin^2\left(\frac{\pi}{n+1}\right)}{\cos\left(\frac{\pi}{n+1}\right) - \cos\left(\frac{2\pi}{n+1}\right)}\,||b|-|c|| \\
&= \frac{n-1}{n+1}\frac{4\sin^2\left(\frac{\pi}{2(n+1)}\right)\cos^2\left(\frac{\pi}{2(n+1)}\right)}{2\sin\left(\frac{3\pi}{2(n+1)}\right)\sin\left(\frac{\pi}{2(n+1)}\right)}\,||b|-|c||
\end{aligned}$$

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A publication of the International Linear Algebra Society
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$$= 2\frac{n-1}{n+1}\frac{\sin\left(\frac{\pi}{2(n+1)}\right)}{\sin\left(\frac{3\pi}{2(n+1)}\right)}\cos^2\left(\frac{\pi}{2(n+1)}\right)||b|-|c||$$

$$\leq 2\frac{n-1}{n+1}1\cdot 1\,||b|-|c|| \leq \sqrt{\frac{n-1}{2}}||b|-|c|| < \sqrt{n-1}||b|-|c||.$$

This proves items (i) and (iii). For item (ii), observe that

$$\sqrt{n_{2,T_n(c,b,a)}(\lambda_k)} = \sqrt{B(n)}||b|-|c|| < \sqrt{\frac{n-1}{2}}||b|-|c|| < \sqrt{n-1}||b|-|c||. \qquad \square$$

5. An example. Consider the matrices $T_7 = T_7(3-4\mathrm{i}, 2+3\mathrm{i}, 0)$ and $T_{30} = T_{30}(3-4\mathrm{i}, 2+3\mathrm{i}, 0)$. The notation T_7 and T_{30} is for the sake of brevity. Here $|b| = \sqrt{13}$ and $|c| = 5$. Evaluating, $\frac{||b|-|c||}{|b|+|c|}\sqrt{\frac{B(n)}{A(n)}}$ for both matrices yields

$$\frac{5-\sqrt{13}}{5+\sqrt{13}}\sqrt{\frac{6}{8}}\frac{\sin\left(\frac{\pi}{8}\right)}{\cos\left(\frac{\pi}{8}\right)-\cos\left(\frac{2\pi}{8}\right)} = 0.2477 < \frac{1}{2}, \quad \text{for } T_7,$$

and

$$\frac{5-\sqrt{13}}{5+\sqrt{13}}\sqrt{\frac{29}{31}}\frac{\sin\left(\frac{\pi}{31}\right)}{\cos\left(\frac{\pi}{31}\right)-\cos\left(\frac{2\pi}{31}\right)} = 1.0337 > \frac{1}{2}, \quad \text{for } T_{30}.$$

According to Propositions 3.1 and 3.2 , T_7 has two shell extremal eigenvalues, namely

$$\lambda_1 = 2\sqrt{((3-4\mathrm{i})(2+3\mathrm{i}))}\cos\left(\frac{\pi}{8}\right) = 7.8424 + 0.2177\mathrm{i} = -\lambda_7,$$

and T_{30} has none. This can also be verified by the graphs of the functions $D(e^{\mathrm{i}\theta}T_7)$ and $D(e^{\mathrm{i}\theta}T_{30})$ in Fig. 1. Calculating the angular sets of Proposition 3.6 for T_7, that is the $\theta \in [0, 2\pi]$ such that $D(e^{\mathrm{i}\theta}T_7) > 0$ (see also Fig. 1), we have

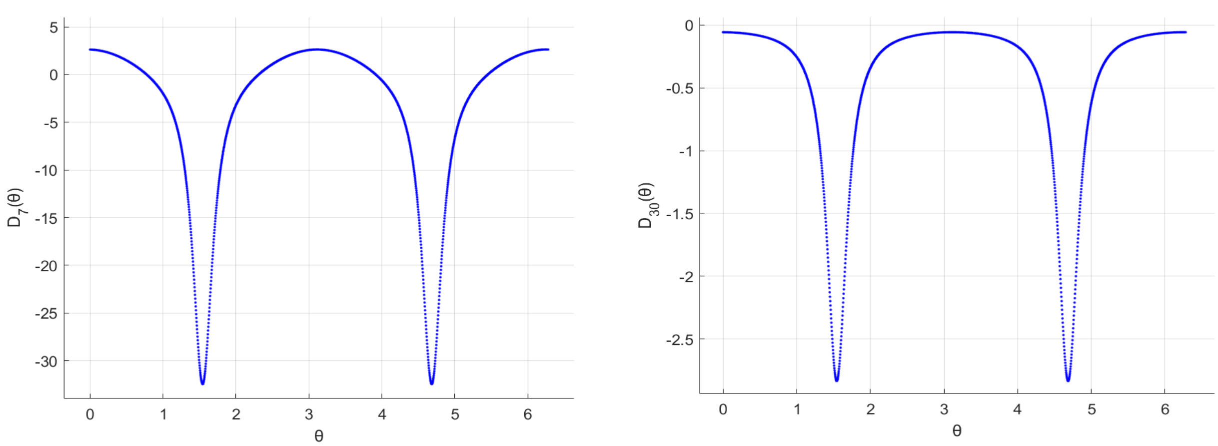

FIGURE 1. *The functions* $D(e^{\mathrm{i}\theta}T_7(3-4\mathrm{i}, 2+2\mathrm{i}, 0))$ *and* $D(e^{\mathrm{i}\theta}T_{30}(3-4\mathrm{i}, 2+3\mathrm{i}, 0))$. $T_7(3-4\mathrm{i}, 2+3\mathrm{i}, 0)$ *has two shell extremal eigenvalues and their corresponding angular sets are formed by the zeroes of* $D(e^{\mathrm{i}\theta}T_7(3-4\mathrm{i}, 2+3\mathrm{i}, 0))$. $D(e^{\mathrm{i}\theta}T_{30}(3-4\mathrm{i}, 2+3\mathrm{i}, 0))$ *is negative for all* $\theta \in [0, 2\pi]$ *verifying that the matrix has no shell extremal eigenvalues.*

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A publication of the International Linear Algebra Society
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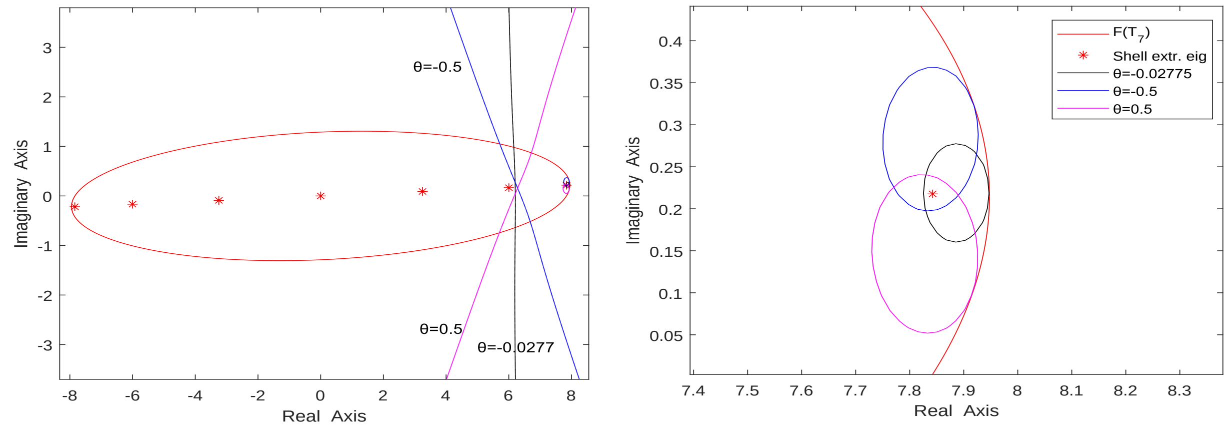

Figure 2. *The curves* $e^{-\mathrm{i}\theta}\Gamma(e^{\mathrm{i}\theta}T_7(3-4\mathrm{i},2+2\mathrm{i},0))$ *for* $\theta=-0.5,-0.02775,0.5$ *(on the left), and on the right a magnified version illustrating the closed branches of these shells that surround the shell extremal eigenvalue* $\lambda_1=7.8424+0.2177\mathrm{i}$*. The convex curve in red is the boundary of the numerical range* $F(T_7(3-4\mathrm{i},2+2\mathrm{i},0))$ *which shares common boundary points with the loops of the shells.*

$$\mathcal{A}(\lambda_1)=[0,0.7758)\cup(5.4519,2\pi)\ \text{ and }\ \mathcal{A}(\lambda_7)=(2.3103,3.9174).$$

This can be verified by evaluating the quantities involved in Proposition 3.6. So,

$$r_2=-\frac{|b|^2+|c|^2}{2|bc|}+\frac{\left||b|^2-|c|^2\right|}{|bc|}\sqrt{\frac{B(n)}{A(n)}}=-\frac{38}{10\sqrt{13}}+\frac{12}{5\sqrt{13}}\sqrt{\frac{6}{8}}\frac{\sin\left(\frac{\pi}{8}\right)}{\cos\left(\frac{\pi}{8}\right)-\cos\left(\frac{2\pi}{8}\right)}=-0.0363,$$

$$\arccos(r_2)=1.6071\quad\text{and}\quad\frac{\theta_b+\theta_c}{2}=\frac{\arg(2+3\mathrm{i})+\arg(3-4\mathrm{i})}{2}=0.0277.$$

Therefore,

$$\theta_1=\left(-\frac{\arccos(r_2)}{2}-\frac{\theta_b+\theta_c}{2}\right)\bmod 2\pi=5.4519\ \text{ and }\ \theta_2=\left(\frac{\arccos(r_2)}{2}-\frac{\theta_b+\theta_c}{2}\right)\bmod 2\pi=0.7758.$$

It is a matter of simple calculations to see that $\mathcal{A}(\lambda_1)=(\theta_1,2\pi)\cup[0,\theta_2)$ and that $\mathcal{A}(\lambda_2)=((\pi+\theta_1)\bmod 2\pi,\pi+\theta_2)$, verifying Proposition 3.6.

Next, in Fig. 2 we draw the shells $e^{-\mathrm{i}\theta}\Gamma(e^{\mathrm{i}\theta}T_7)$ for $\theta=-0.5$, $\theta=-\dfrac{\theta_b+\theta_c}{2}=-0.02775$ and $\theta=0.5$ and in Table 1 we evaluate the related quantities $D(e^{\mathrm{i}\theta}T_7)$, $\nu(e^{\mathrm{i}\theta}T_7)-u(e^{\mathrm{i}\theta}T_7)^2$, $d_h(e^{\mathrm{i}\theta}T_7)$ and $R_{\Gamma(e^{\mathrm{i}\theta}T_7)}(\delta_1(e^{\mathrm{i}\theta}T_7)+\mathrm{i}u(e^{\mathrm{i}\theta}T_7))$. The last three quantities attain their minima at $\theta=-0.02775$ as Proposition 4.1 requires. To verify this, we calculate the quantities $n_i(T_7)$ $i=1,2,3$. Note that $A(7)=\left(\cos\left(\frac{\pi}{8}\right)-\cos\left(\frac{2\pi}{8}\right)\right)^2=0.0470$ and $B(7)=\dfrac{6}{8}\sin^2\left(\frac{\pi}{8}\right)=0.1098$. So,

$$n_1(T_7(3-4\mathrm{i},2+3\mathrm{i},0))=\frac{1}{2}\left(\sqrt{(|b|+|c|)^2A(n)}-\sqrt{(|b|+|c|)^2A(n)-4B(n)(|b|-|c|)^2}\right)=0.1225,$$

$$n_2(T_7(3-4\mathrm{i},2+3\mathrm{i},0))=B(n)(|b|-|c|)^2=0.2136\ \text{ and }\ n_3(T_7(3-4\mathrm{i},2+3\mathrm{i}))=\frac{B(n)(|b|-|c|)^2}{2\sqrt{A(n)}(|b|+|c|)}=0.0572.$$

Moreover,

Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 39, pp. 572-590, November 2023.

TABLE 1
The values of $D(e^{i\theta}T_7)$, $\nu(e^{i\theta}T_7) - u(e^{i\theta}T_7)^2$, $d_h(e^{i\theta}T_7)$ *and* $R_{\Gamma(e^{i\theta}T_7)}(\delta_1(e^{i\theta}T_7) + iu(e^{i\theta}T_7))$ *at* $\theta = -0.5, -0.02775, 0.5$.

θ	-0.5	-0.02775	0.5
$D(e^{i\theta}T_7)$	1.7089	2.6256	1.4861
$\nu(e^{i\theta}T_7) - u(e^{i\theta}T_7)^2$	0.2675	0.2136	0.2836
$d_h(e^{i\theta}T_7)$	0.1799	0.1225	0.1999
$R_{\Gamma(e^{i\theta}T_7)}(\delta_1(e^{i\theta}T_7) + iu(e^{i\theta}T_7))$	0.0802259	0.0572443	0.0875975

$$\Delta_F(T_7(3-4i, 2+3i, 0)) = \sqrt{6}(5-\sqrt{13}) = 3.4157 \text{ and } \delta_F(T_7(3-4i, 2+3i, 0)) = \sqrt{3}(5-\sqrt{13}) = 2.4153.$$

We can also see that the inequalities of Corollary 4.4 are satisfied.

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