ON THE INVERSE PROBLEM OF CONSTRUCTING SYMMETRIC PENTADIAGONAL TOEPLITZ MATRICES FROM THREE LARGEST EIGENVALUES

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Abstract. The inverse problem of constructing a symmetric Toeplitz matrix with prescribed eigenvalues has been a challenge both theoretically and computationally in the literature. It is now known in theory that symmetric Toeplitz matrices can have arbitrary real spectra. This paper addresses a similar problem — Can the three largest eigenvalues of symmetric pentadiagonal Toeplitz matrices be arbitrary? Given three real numbers $\nu \leq \mu \leq \lambda$, this paper finds that the ratio $\alpha = \frac{\lambda-\nu}{\mu-\nu}$, including infinity if $\mu = \nu$, determines whether there is a symmetric pentadiagonal Toeplitz matrix with ν, μ, and λ as its three largest eigenvalues. It is shown that such a matrix of size $n \times n$ does not exist if n is even and α is too large, or if n is odd and α is too close to one. When such a matrix does exist, a numerical method is proposed for the construction.

Key words. inverse eigenvalue problem, pentadiagonal matrices, Toeplitz matrices, eigenvalue inequalities

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1. Introduction.

The inverse eigenvalue problem concerns finding a matrix with a specified structure and a prescribed spectrum. One of its variations is the Toeplitz inverse eigenvalue problem where a symmetric Toeplitz matrix is to be constructed with prescribed spectrum. A $n \times n$ symmetric Toeplitz matrix is completely characterized by its first row. We denote this fact by $toeplitz([z_1, \ldots, z_n])$. It thus seems reasonable to expect that the n entries of the first row could be determined from n given eigenvalues. This seemingly simple existence question, however, had intrigued researchers for decades before a formal proof of its solvability was settled by Landau via a topological degree argument [10]. The nonconstructive proof shows that every set of n real numbers can be the spectrum of a certain $n \times n$ real symmetric *regular* Toeplitz matrix. Numerical construction of such a matrix remains to be a challenging task despite many efforts in the literature [4, 5, 7, 16, 17].

This paper deals with a related but different inverse problem — Can a real, symmetric, and pentadiagonal Toeplitz matrix have three arbitrary largest eigenvalues? Such a question is not only of theoretical interest but also of practical importance because banded Toeplitz structure arises frequently in applications [1, 2, 6, 14] and for large-scale problems often the first few extreme eigenvalues are critical [12, 18].

As will be seen in the subsequent discussion, the restriction of the prescribed eigenvalues to the largest three in the spectrum indeed helps to establish the existence theory. Without this restriction, the problem would be harder to handle. The question of whether $n \times n$ symmetric and pentadiagonal Toeplitz matrices can have three arbitrary real numbers as eigenvalues, not necessarily in any specified order, is of interest in its own right, but is not the focus of this paper. The more general question of whether $n \times n$ symmetric and banded Toeplitz matrices $toeplitz([z_1, \ldots, z_k, 0, \ldots, 0])$ can have k arbitrary real numbers as eigenvalues, not necessarily in any specified order, appears even more difficult to answer. Given Landau's result that $n \times n$ symmetric Toeplitz matrix $toeplitz([z_1, \ldots, z_n])$ can have n arbitrary eigenvalues, our result that $n \times n$ symmetric Toeplitz matrix $toeplitz([z_1, z_2, z_3, 0, \ldots, 0])$ with $n > 3$ cannot have three arbitrary largest eigenvalues seems new and surprising.

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It is well known that the spectrum of the $n \times n$ symmetric and tridiagonal Toeplitz matrix $toeplitz([a, b, 0, \ldots 0])$ consists of values

$$\mu_{n+1-k} = a + 2b \cos \frac{k\pi}{n+1}, \quad k = 1, \ldots n. \tag{1.1}$$

Given any two arbitrary real values $\mu_{n-1} < \mu_n$, it is clear that, because the cosine function is strictly decreasing over the interval $(0, \pi)$, values a and b can be found so that $toeplitz([a, b, 0, \ldots 0])$ has $\{\mu_{n-1}, \mu_n\}$ as its first two largest eigenvalues. Once a and b are fixed, the third largest eigenvalue μ_{n-2} is necessarily determined.

Throughout this note, let $A_n := A_n(a, b, c)$ denote the $n \times n$ symmetric and pentadiagonal Toeplitz matrix

$$A_n(a, b, c) := toeplitz([a, b, c, 0, ..., 0]). \tag{1.2}$$

Without loss of generality, we shall rule out the case $c = 0$. For reasons that will become clear later, we shall also assume temporarily that $c > 0$. Let $B_n = B_n(\gamma)$ denote the associate matrix,

$$B_n(\gamma) := toeplitz([0, \gamma, 1, 0, ..., 0]), \tag{1.3}$$

where $\gamma := b/c$. Assume that all eigenvalues are arranged in ascending order, that is, $\lambda_1(A_n) \leq \ldots \leq \lambda_n(A_n)$ and so on. It is obvious that eigenvalues $\lambda_i(A_n)$ of A_n are related to eigenvalues $\lambda_i(B_n)$ via the relationship

$$a + c\lambda_i(B_n) = \lambda_i(A_n). \tag{1.4}$$

It follows that, from given any two sets of eigenvalues $\{\lambda_i(A_n), \lambda_j(A_n)\}$ and $\{\lambda_i(B_n), \lambda_j(B_n)\}$, we can solve

$$a = \frac{\lambda_j(B_n)\lambda_i(A_n) - \lambda_i(B_n)\lambda_j(A_n)}{\lambda_j(B_n) - \lambda_i(B_n)}, \tag{1.5}$$

$$c = \frac{\lambda_j(A_n) - \lambda_i(A_n)}{\lambda_j(B_n) - \lambda_i(B_n)}, \tag{1.6}$$

provided $\lambda_j(B_n) \neq \lambda_i(B_n)$. Plugging in a and c for any other $\lambda_k(B_n)$, we see that

$$\lambda_k(B_n) = \alpha\lambda_j(B_n) + (1 - \alpha)\lambda_i(B_n), \tag{1.7}$$

with

$$\alpha = \frac{\lambda_k(A_n) - \lambda_i(A_n)}{\lambda_j(A_n) - \lambda_i(A_n)}. \tag{1.8}$$

The inverse eigenvalue problem for the symmetric and pentadiagonal Toeplitz matrix A_n therefore can be reformulated as follows:

> *Given three (largest) eigenvalues $\lambda_i(A_n) < \lambda_j(A_n) < \lambda_k(A_n)$ of A_n, find the scalar γ such that $B_n(\gamma)$ has three eigenvalues $\lambda_i(B_n) < \lambda_j(B_n) < \lambda_k(B_n) = \alpha\lambda_j(B_n) + (1 - \alpha)\lambda_i(B_n)$ with α defined by (1.8).*

We shall refer to this problem as *the inverse problem for the matrix $B_n(\gamma)$*.

The difference quotient relationship,

$$\frac{\lambda_k(A_n) - \lambda_i(A_n)}{\lambda_j(A_n) - \lambda_i(A_n)} = \frac{\lambda_k(B_n) - \lambda_i(B_n)}{\lambda_j(B_n) - \lambda_i(B_n)} = \alpha, \tag{1.9}$$

between three ordered eigenvalues of A_n and B_n follows from (1.7). Observe the clear advantage that there is only one free parameter γ involved in the matrix $B_n(\gamma)$. Our understanding about the spectrum of the simpler $B_n(\gamma)$ will shed considerable insights into the inverse eigenvalue problem for the A_n by using the relationship (1.9) as we explain below.

2. Preliminaries. While the spectra of $B_{2n}(\gamma)$ and $B_{2n-1}(\gamma)$ share many similar properties, the even or odd dimensionality does have different effect on the solvability of the inverse problem. To prepare for the investigation, we first introduce some fundamental facts about the spectrum of $B_n(\gamma)$ in general. A series of results that eventually build up the answer to the question of solvability for the inverse problem of pentadiagonal Toeplitz matrix with three prescribed largest eigenvalues will be derived in the sequel. We believe that some of the results presented in this section are new and are of interest in their own right.

By writing $\frac{B_n(\gamma)}{\gamma} = toeplitz([0, 1, 1/\gamma, 0, \ldots, 0])$ and using (1.1), the following asymptotic behavior is clear.

LEMMA 2.1. *Let the eigenvalues $\lambda_1(B_n(\gamma)) \leq \ldots \leq \lambda_n(B_n(\gamma))$ be arranged in increasing order. Then*

$$\lim_{\gamma \to \pm\infty} \frac{\lambda_{n+1-k}(B_n(\gamma))}{\gamma} = \pm 2 \cos \frac{k\pi}{n+1}, \quad k = 1, \ldots, n. \tag{2.1}$$

There is a recursive relation for the determinant of a pentadiagonal matrix [15]. In particular, denote the characteristic polynomial of A_k by

$$\rho_k = \rho_k(\lambda; a, b, c) := \det(A_k - \lambda I), \tag{2.2}$$

then the following fact can be derived.

THEOREM 2.2. *Define $\rho_{-1} := 0$, $\rho_0 := 1$, $\rho_1 := a - \lambda$, $\rho_2 := (a-\lambda)^2 - b^2$, and $\rho_3 := (a-\lambda)^3 - 2(a-\lambda)b^2 + 2cb^2 - (a-\lambda)c^2$. Then for $k = 4, 5, \ldots$, the polynomial ρ_k satisfies a 6-term recursion relationship*

$$\begin{aligned}\rho_k := (a-\lambda-c)\,\rho_{k-1} - \left(b^2 - (a-\lambda)\,c\right)\rho_{k-2} - \left((a-\lambda)\,c^2 - b^2 c\right)\rho_{k-3} \\ +c^2\left(c^2 - (a-\lambda)\,c\right)\rho_{k-4} + c^5 \rho_{k-5}.\end{aligned} \tag{2.3}$$

Let the characteristic polynomial of $B_k(\gamma)$ be noted by

$$\varrho_k = \varrho_k(\lambda; \gamma) = \det(B_k - \lambda I).$$

With $\varrho_{-1} := 0$, $\varrho_0 := 1$, $\varrho_1 := -\lambda$, $\varrho_2 := \lambda^2 - \gamma^2$, and $\varrho_3 := -\lambda^3 + 2\lambda\gamma^2 + 2\gamma^2 + \lambda$, we see from the above theorem that for $k \geq 4$, ϱ_k is given recursively by

$$\varrho_k = -(1+\lambda)\,\varrho_{k-1} - \left(\gamma^2 + \lambda\right)\varrho_{k-2} + \left(\gamma^2 + \lambda\right)\varrho_{k-3} + (1+\lambda)\,\varrho_{k-4} + \varrho_{k-5},$$

which clearly is an even function in γ.

COROLLARY 2.3. *Both $B_n(\gamma)$ and $B_n(-\gamma)$ have the same characteristic polynomial and, hence, the same set of eigenvalues.*

Additional symmetry on the eigenvalues of $B_n(\gamma)$ can be obtained from exploiting its centrosymmetric structure. We shall demonstrate the case for B_{2n} only. A similar argument can be carried out for $B_{2n-1}(\gamma)$. Let $\Xi_n = [\xi_{ij}]$ denote the $n \times n$ standard involution permutation matrix, that is, the perdiagonal matrix whose entries are defined by

$$\xi_{ij} = \begin{cases} 1 & \text{if } i = n+1-j, \\ 0 & \text{otherwise.} \end{cases}$$

Any $2n \times 2n$ centrosymmetric matrix M_{2n} is of the form [3]

$$M_{2n} = \begin{bmatrix} X_n & Y_n^\top \\ Y_n & \Xi_n X_n \Xi_n \end{bmatrix},$$

where $X_n, Y_n \in \mathbb{R}^{n\times n}$ and X_n is symmetric. Define the orthogonal matrix

$$K_{2n} := \frac{1}{\sqrt{2}} \begin{bmatrix} I_n & -\Xi_n \\ I_n & \Xi_n \end{bmatrix},$$

where I_n is the $n \times n$ identity matrix. It is not difficult to see that

$$K_{2n} M_{2n} K_{2n}^T = \begin{bmatrix} X_n - \Xi_n Y_n & 0 \\ 0 & X_n + \Xi_n Y_n \end{bmatrix}.$$

The spectra of $X_n \mp \Xi_n Y_n$ are known as eigenvalues of M_{2n} with *odd* and *even* parity, respectively. Upon applying the same orthogonal similarity transformation to $M_{2n} = B_{2n}(\gamma)$ of size $2n \times 2n$, we observe the structure where the corresponding $n \times n$ matrices $X_n \mp \Xi_n Y_n$ of $B_{2n}(\gamma)$ are of the form

$$\begin{bmatrix} 0 & \gamma & 1 & 0 & \dots & & & & 0 \\ \gamma & 0 & \gamma & 1 & & & & & 0 \\ 1 & \gamma & 0 & \gamma & & & & & \\ & & & & \ddots & & & & \\ & & & & \ddots & & & & \\ & & & & & & \gamma & 1 & 0 \\ & & & & & \gamma & 0 & \gamma & 1 \\ 0 & & & & & 1 & \gamma & 0 & \gamma \mp 1 \\ 0 & 0 & 0 & & & 0 & 1 & \gamma \mp 1 & \mp\gamma \end{bmatrix}, \tag{2.4}$$

respectively. Let

$$\begin{aligned} f(\lambda;\gamma) &:= \det(X_n - \Xi_n Y_n - \lambda I), \\ g(\lambda;\gamma) &:= \det(X_n + \Xi_n Y_n - \lambda I), \end{aligned}$$

denote the characteristic polynomials of $X_n \mp \Xi_n Y_n$, respectively. Then it is easy to see that $f(\lambda;\gamma) = g(\lambda;-\gamma)$. A similar argument can be applied to $B_{2n-1}(\gamma)$. We therefore have proved another spectral property of B_n.

Lemma 2.4. *The very same eigenvalue of $B_{2n}(\gamma)$ and $B_{2n}(-\gamma)$ has opposite parity whereas the very same eigenvalue of $B_{2n-1}(\gamma)$ and $B_{2n-1}(-\gamma)$ maintains the same parity.*

By the symmetry described in Corollary 2.3 and Lemma 2.4, it suffices to consider for our inverse problem the case $\gamma \geq 0$ only. The inverse problem is solvable for some γ if and only if it is solvable for some $\gamma \geq 0$ and, in this case, it is also solvable for $-\gamma$. Furthermore, the eigenstructure of the matrix $B_n(0)$ for the special case of $\gamma = 0$ is easy. Indeed, let the Gauss brackets $\lceil\cdot\rceil$ and $\lfloor\cdot\rfloor$ denote the smallest integer greater than and the largest integer not greater than the number they embrace, respectively. Then $B_n(0)$ can be effectively reduced by permutations to two tridiagonal Toeplitz matrices *toeplitz*$([0, 1, 0, \dots, 0])$ of size $\lceil n/2\rceil$ and $\lfloor n/2\rfloor$, respectively, whose eigenvalues are known according to (1.1).

Lemma 2.5. *The eigenvalues of $B_{2n-1}(0)$ are all simple and, if listed in ascending order, alternate the parities with the largest eigenvalue even. Each eigenvalue of $B_{2n}(0)$ is always a double eigenvalue.*

Henceforth, we shall limit our attention to the case $\gamma > 0$ only. Immediately, we find that the largest eigenvalue has the following characteristics.

Theorem 2.6. *If $\gamma > 0$, then the largest eigenvalue of $B_n(\gamma)$ is positive, simple, and has an even parity.*

Proof. Since $\gamma > 0$, the matrix $B_n(\gamma)$ is irreducible and nonnegative. The well-known Perron-Frobenius Theorem [8, Theorem 8.4.4] asserts that the spectral radius of $B_n(\gamma)$ is precisely the largest eigenvalue $\lambda_n(B_n(\gamma))$ of $B_n(\gamma)$ and that $\lambda_n(B_n(\gamma))$ is simple. The corresponding eigenvector is necessarily of one sign and, hence, must be an even vector. ∎

For later reference, we recall a special case of the well-known Courant-Fischer Theorem. The condition where equalities hold is of particular importance to us.

THEOREM 2.7. *Let $P \in \mathbb{R}^{n\times m}$ be such that $P^\top P = I_m$. Let $S \in \mathbb{R}^{n\times n}$ be symmetric and define $T := P^\top SP$. Let the spectra of S and T be denoted as $\theta_1 \leq \ldots \leq \theta_n$ and $\tau_1 \leq \ldots \leq \tau_m$, respectively. Then the interlacing property*

$$\theta_j \leq \tau_j \leq \theta_{n-m+j}$$

holds for $1 \leq j \leq m$. If $\theta_j = \tau_j$ for some j, then there exists a vector $\mathbf{v} \in \mathbb{R}^m$ such that

$$\begin{aligned} T\mathbf{v} &= \tau_j \mathbf{v}, \\ SP\mathbf{v} &= \theta_j P\mathbf{v}. \end{aligned}$$

Proof. The fact that the spectra of S and T interlace with each other can be found in many references. See, for example, [8, Theorem 4.2.1]. For completion, however, we briefly outline the proof with emphasis on the case when one of the equalities hold.

Let $\{\mathbf{u}_1, \ldots, \mathbf{u}_n\}$ be an orthonormal basis of eigenvectors of S and let $\{\mathbf{v}_1, \ldots, \mathbf{v}_m\}$ be such a basis for T. Denote the invariant subspaces spanned by $\{\mathbf{u}_1, \ldots, \mathbf{u}_i\}$ and by $\{\mathbf{v}_1, \ldots, \mathbf{v}_j\}$ by U_i and V_j, respectively. It is clear that, given any $\mathbf{u} \in U_{j-1}^\perp$ and $\mathbf{v} \in V_j$,

$$\mathbf{v}^\top T\mathbf{v} \leq \tau_j \mathbf{v}^\top \mathbf{v}, \tag{2.5}$$

$$\mathbf{u}^\top S\mathbf{u} \geq \theta_j \mathbf{u}^\top \mathbf{u}. \tag{2.6}$$

Suppose that the equality in (2.5) holds. Write $\mathbf{v} = \sum_{i=1}^j \xi_i \mathbf{v}_i$. Then

$$\tau_j \sum_{i=1}^j \xi_i^2 = \mathbf{v}^\top T\mathbf{v} = \sum_{i=1}^j \xi_i^2 \tau_i \leq \tau_{j-1} \sum_{i=1}^{j-1} \xi_i^2 + \tau_j \xi_j^2.$$

It follows that either $\sum_{i=1}^{j-1} \xi_i^2 = 0$ or $\tau_j = \tau_{j-1}$. In the former, $\mathbf{v}$ is parallel to $\mathbf{v}_j$ and, hence, is an eigenvector. In the latter, we can replace the inequality by

$$\tau_j \sum_{i=1}^j \xi_i^2 = \mathbf{v}^\top T\mathbf{v} = \sum_{i=1}^j \xi_i^2 \tau_i \leq \tau_{j-2} \sum_{i=1}^{j-2} \xi_i^2 + \tau_j \xi_{j-1}^2 + \tau_j \xi_j^2.$$

We thus conclude that either $\mathbf{v}$ belongs to the eigenspace spanned by $\{\mathbf{v}_{j-1}, \mathbf{v}_j\}$ or $\tau_j = \tau_{j-1} = \tau_{j-2}$. The process can be continued and must terminate in finitely many steps. In all cases, $\mathbf{v}$ is an eigenvector corresponding to the eigenvalue τ_j. Similarly, if the equality in (2.6) holds, then $\mathbf{u}$ must be an eigenvector corresponding to the eigenvalue θ_j.

It is clear that the subspace $V_j \bigcap (P^\top U_{j-1})^\perp \subset \mathbb{R}^m$ is of dimension at least one. Let $\mathbf{v}$ be a nonzero vector in $V_j \bigcap (P^\top U_{j-1})^\perp$. Then it must be the case that $P\mathbf{v} \in U_{j-1}^\perp$. It follows that

$$\theta_j \leq \frac{\mathbf{v}^\top P^\top SP\mathbf{v}}{\mathbf{v}^\top P^\top P\mathbf{v}} = \frac{\mathbf{v}^\top T\mathbf{v}}{\mathbf{v}^\top \mathbf{v}} \leq \tau_j.$$

In the event that $\theta_j = \tau_j$ for some j, we see that the vector $\mathbf{v} \in V_j \bigcap (P^\top U_{j-1})^\perp$ is an eigenvector of T with eigenvalue τ_j and $P\mathbf{v}$ is an eigenvector of S with eigenvalue θ_j.

By applying a similar argument, the other inequality can be established. In particular, there exists a nonzero vector $\mathbf{v} \in V_{j-1}^{\perp} \bigcap (P^{\top} U_{n-m+j}^{\perp})^{\perp}$ such that

$$\tau_j \leq \frac{\mathbf{v}^{\top} T \mathbf{v}}{\mathbf{v}^{\top} \mathbf{v}} = \frac{\mathbf{v}^{\top} P^{\top} S P \mathbf{v}}{\mathbf{v}^{\top} P^{\top} P \mathbf{v}} \leq \theta_{n-m+j}.$$

If $\theta_{n-m+j} = \tau_j$ for some j, we see that the vector $\mathbf{v} \in V_{j-1}^{\perp} \bigcap (P^{\top} U_{n-m+j}^{\perp})^{\perp}$ is an eigenvector of T with eigenvalue τ_j and $P\mathbf{v} \in U_{n-m+j}$ is an eigenvector of S with eigenvalue θ_{n-m+j}. ∎

It is not difficult to calculate that the second largest eigenvalue of $B_4(\gamma)$ is given by

$$\lambda_3(B_4(\gamma)) = \frac{\sqrt{5\gamma^2 - 8\gamma + 4} - \gamma}{2}.$$

By the interlacing property, we know that $\lambda_{k-1}(B_k(\gamma)) \geq \lambda_3(B_4(\gamma))$ for all $k \geq 4$. We thus confirm the nonnegativity of the second largest eigenvalue.

LEMMA 2.8. *For $k \geq 4$, the second largest eigenvalue $\lambda_{k-1}(B_k(\gamma))$ is always nonnegative.*

We next address the algebraic multiplicity of eigenvalues of $B_n(\gamma)$.

THEOREM 2.9. *If $\gamma > 0$, then any eigenvalue of the matrix $B_n(\gamma)$ can have multiplicity at most two.*

Proof. We shall prove the result by induction. Eigenvalues of $B_3(\gamma)$ are -1 and $\frac{1 \pm \sqrt{1+8\gamma^2}}{2}$. It is clear that any eigenvalue can have multiplicity at most two.

Assume that the assertion is true for $B_\ell(\gamma)$. Let $\{\mathbf{u}_1, \ldots, \mathbf{u}_{\ell+1}\}$ be an orthonormal basis of eigenvectors corresponding to eigenvalues $\{\theta_1, \ldots, \theta_{\ell+1}\}$ of $B_{\ell+1}$. Likewise, let $\{\mathbf{v}_1, \ldots, \mathbf{v}_\ell\}$ be such a basis for B_ℓ with eigenvalues $\{\tau_1, \ldots, \tau_\ell\}$. Denote the invariant subspaces spanned by $\{\mathbf{u}_1, \ldots, \mathbf{u}_i\}$ and by $\{\mathbf{v}_1, \ldots, \mathbf{v}_j\}$ by U_i and V_j, respectively. By Theorem 2.7, the interlacing relationship

$$\theta_{j-1} \leq \tau_{j-1} \leq \theta_j \leq \tau_j \leq \theta_{j+1}$$

holds for all $1 \leq j \leq \ell$.

Suppose that for some j, $\theta_{j-1} = \theta_j = \theta_{j+1}$. Then using arguments given in the proof of Theorem 2.7, we are certain that there exist eigenvectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^\ell$ of $B_\ell(\gamma)$ from the subspaces

$$\mathbf{x} \in V_{j-1} \bigcap (P^{\top} U_{j-2})^{\perp},$$
$$\mathbf{y} \in V_{j-1}^{\perp} \bigcap (P^{\top} U_{j+1}^{\perp})^{\perp},$$

respectively, such that $[\mathbf{x}^{\top}, 0]^{\top}, [\mathbf{y}^{\top}, 0]^{\top} \in \mathbb{R}^{\ell+1}$ are eigenvectors of $B_{\ell+1}(\gamma)$. It follows that $\mathbf{x} \perp \mathbf{y}$ and, hence, are linearly independent. By assumption, any other eigenvector of $B_\ell(\gamma)$ with eigenvalue τ_j must be a linear combination of $\mathbf{x}$ and $\mathbf{y}$, and vice versa. In particular, $\Xi_\ell \mathbf{x}$ and $\Xi_\ell \mathbf{y}$ are also eigenvectors of $B_\ell(\gamma)$. Without loss of generality, we may now assume that $\mathbf{x}$ is an even vector and $\mathbf{y}$ is an odd vector. It then follows that both $\mathbf{x}$ and $\mathbf{y}$ have nonzero first entries.

Recall that $\Xi_{\ell+1} B_{\ell+1}(\gamma) \Xi_{\ell+1} = B_{\ell+1}(\gamma)$. It follows that all four vectors

$$\begin{bmatrix} \mathbf{x} \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ \mathbf{x} \end{bmatrix}, \quad \begin{bmatrix} \mathbf{y} \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ -\mathbf{y} \end{bmatrix},$$

are eigenvectors of $B_{\ell+1}$. With the fact that $\mathbf{x} \perp \mathbf{y}$, it is not difficult to check that these four vectors are necessarily independent, implying that θ_j is of multiplicity at least four. By the interlacing property, it would imply that τ_j is of multiplicity at least three, contradicting with the assumption in the induction. ∎

Note that the family of matrices $B_n(\gamma)$ depends analytically on the parameter γ, it is a classical result that $B_n(\gamma)$ enjoys an analytic Schur decomposition [9, 13]. In particular, at any simple eigenvalue λ_0 of $B_n(\gamma_0)$ there exists a neighborhood of γ_0 in which both the eigenvalue $\lambda(\gamma)$ and the corresponding unit eigenvector $\mathbf{v}(\gamma)$ are analytic in γ. It is easy to see that the eigenvalue curve $\lambda(\gamma)$ satisfies the initial value problem

$$\frac{d\lambda(\gamma)}{d\gamma} = \mathbf{v}(\gamma)^\top C\mathbf{v}(\gamma), \quad \lambda(\gamma_0) = \lambda_0 \tag{2.7}$$

where $C := \mathit{toeplitz}([0,1,0,\dots,0])$. This differential equation relationship remains valid even if λ_0 is a multiple eigenvalue. Indeed, if $\{\epsilon_m\}$ is a sequence of nonzero real numbers tending to 0 for which $\lim_{m\to\infty} \mathbf{v}(\gamma_0+\epsilon_m) = \mathbf{u}(\gamma_0)$ exists, then the limit

$$\lim_{m\to\infty} \frac{\lambda(\gamma_0+\epsilon_m)-\lambda(\gamma_0)}{\epsilon_m} = \mu(\gamma_0)$$

also exists [13, Page 45]. In this case, it can be proved that $B_n(\gamma_0)\mathbf{u}(\gamma_0) = \lambda_0\mathbf{u}(\gamma_0)$ and $\mu(\gamma_0) = \mathbf{u}(\gamma_0)^\top C\mathbf{u}(\gamma_0)$. We claim that these eigenvalue curves intersect transversally at multiple eigenvalues in the following sense.

THEOREM 2.10. *If $\mathbf{x}$ and $\mathbf{y}$ are two orthonormal eigenvectors of $B_n(\gamma_0)$ corresponding to the same eigenvalue λ_0, then $\mathbf{x}^\top C\mathbf{x} \neq \mathbf{y}^\top C\mathbf{y}$.*

Proof. By Theorem 2.9, $\mathbf{x}$ and $\mathbf{y}$ form the basis of the eigenspace Ω corresponding to λ_0 for $B_n(\gamma_0)$. That is, Ω is of dimension two.

Assume that $\mathbf{x}^\top C\mathbf{x} = \mathbf{y}^\top C\mathbf{y} = \alpha$ Then $\mathbf{w}^\top C\mathbf{w} = \alpha$ for every unit vector $\mathbf{w}$ in Ω. Note that $B_n(\gamma) = \gamma C + E$ where $E := \mathit{toeplitz}([0,0,1,0,\dots,0])$. From the fact that $\lambda_0 = \mathbf{x}^\top B_n(\gamma_0)\mathbf{x} = \mathbf{y}^\top B_n(\gamma_0)\mathbf{y}$, we must have $\mathbf{x}^\top E\mathbf{x} = \mathbf{y}^\top E\mathbf{y} = \beta$. This would imply that at every $\gamma \in \mathbb{R}$ it is always the case that $\mathbf{w}^\top B_n(\gamma)\mathbf{w} \equiv \gamma\alpha + \beta$ for every unit vector $\mathbf{w} \in \Omega$, which is not possible . □

For any fixed $\gamma_0 \in \mathbf{R}$, denote

$$a := \mathbf{v}(\gamma_0)^\top C\mathbf{v}(\gamma_0),$$
$$b := \mathbf{v}(\gamma_0)^\top E\mathbf{v}(\gamma_0),$$

where $\mathbf{v}(\gamma_0)$ is the unit eigenvector of $B_n(\gamma_0)$ corresponding to the largest eigenvalue $\lambda_n(B_n(\gamma_0))$. Since

$$\mathbf{u}^\top B_n(\gamma)\mathbf{u} = \gamma\mathbf{u}^\top C\mathbf{u} + \mathbf{u}^\top E\mathbf{u} \le \lambda_n(B_n(\gamma))$$

for all unit vectors $\mathbf{u} \in \mathbf{R}^n$, it follows that

$$a\gamma + b \le \lambda_n(B_n(\gamma)) \tag{2.8}$$

for all $\gamma \in \mathbb{R}$. This inequality (2.8) together with its equality at γ_0 shows that largest eigenvalue curve $\lambda_n(B_n(\gamma))$ of $B_n(\gamma)$ is being supported below by the straight line $y = a\gamma + b$ at γ_0. Indeed, such a support exists at every γ_0. This shows the convexity of $\lambda_n(B_n(\gamma))$. A similar argument can be given for the smallest eigenvalue curve which we summarize as follows [13, Page 42].

LEMMA 2.11. *The largest eigenvalue $\lambda_n(B_n(\gamma))$ is a convex function of γ while the smallest eigenvalue $\lambda_1(B_n(\gamma))$ is a concave function of γ.*

3. Solvability.

The recursive formula (2.3) can be employed as a numerical means to construct a symmetric and pentadiagonal Toeplitz matrix with three prescribed eigenvalues. We will discuss later how the recursion can be compacted into matrix form which facilitates the computation. Before such an endeavor, however, a more fundamental question is whether the inverse problem is solvable. Toward that end, for fixed indices i, j and k, define the subset R_{ijk} of real numbers by

$$R_{ijk} := \left\{ \frac{\lambda_k(B_n) - \lambda_i(B_n)}{\lambda_j(B_n) - \lambda_i(B_n)} | \gamma \in \mathbb{R} \right\}. \tag{3.1}$$

The range of R_{ijk} plays a critical role in the solvability according to the following observation.

THEOREM 3.1. *The inverse eigenvalue problem for A_n is solvable for any eigenvalues $\lambda_i(A_n) < \lambda_j(A_n) < \lambda_k(A_n)$ if and only if $R_{ijk} = [1, \infty)$. If R_{ijk} is bounded in the interval $[\zeta, \eta]$, then the inverse eigenvalue problem is not solvable if*

$$\frac{\lambda_k(A_n) - \lambda_i(A_n)}{\lambda_j(A_n) - \lambda_i(A_n)} > \eta, \quad or \quad \frac{\lambda_k(A_n) - \lambda_i(A_n)}{\lambda_j(A_n) - \lambda_i(A_n)} < \zeta.$$

Proof. The given ordered triplet $\lambda_i(A_n) < \lambda_j(A_n) < \lambda_k(A_n)$ determines a value for α according to (1.8). In the meantime, by (1.9), α is a function of γ. Any value of α in the range of R_{ijk} corresponds to at least one value of γ which, in turn, determines the ordered triplet $\lambda_i(B_n) < \lambda_j(B_n) < \lambda_k(b_n)$. Finally, values of a and c are determined from equations (1.4) and $b = c\gamma$. □

A simple numerical experiment with the case $n = 4$ illustrates the significance of Theorem 3.1. In Figure 3.1, the eigenvalues of $B_4(\gamma) = toeplitz([0, \gamma, 1, 0])$ are plotted against $\gamma \in [-20, 20]$. Many of the properties described earlier are manifested in this figure. The ratio α defined in (1.9)

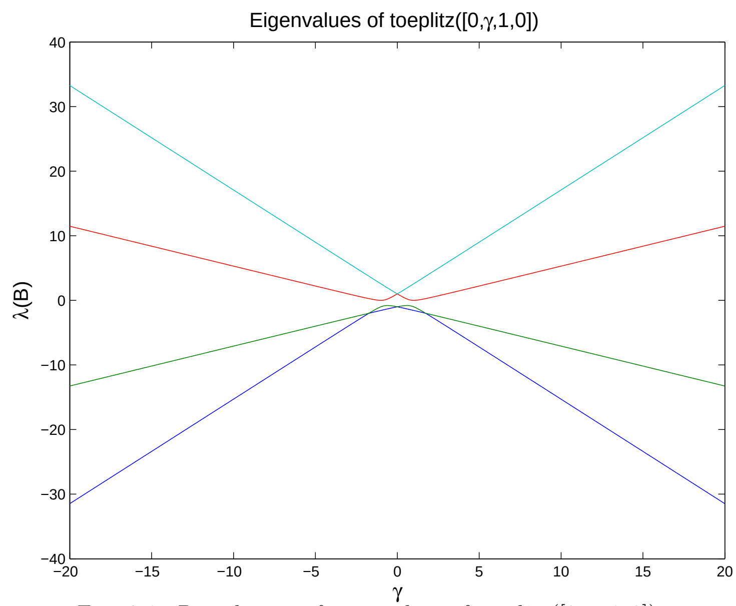

FIG. 3.1. *Distribution of eigenvalues of toeplitz*$([0, \gamma, 1, 0])$.

by the three largest eigenvalues of $B_4(\gamma)$ is plotted in the left drawing in Figure 3.2. It appears that the set R_{234} should be bounded. A test of 500 matrices $A_4 = toeplitz([a, b, c, 0])$ with entries a, b and c randomly generated from the standard normal distribution, depicted in the right drawing of Figure 3.2, seems to reaffirm this observation. Although Landau's result asserts that $\{1, 2, 6\}$ is the spectrum of a certain 3×3 symmetric Toeplitz matrix $toeplitz([a, b, c])$, this experiment seems to suggest that no symmetric Toeplitz matrix $toeplitz([a, b, c, 0])$ can have $\{1, 2, 6\}$ as its three largest eigenvalues because the ratio $\alpha = 5$ is too large. We shall investigate the general case in more details. We separate discussion into two cases.

3.1. Even Dimension. Trivially, the difference quotient α of the three largest eigenvalues of any (symmetric) matrix is at least 1. We know by Lemma 2.5 that this minimal ratio for $B_{2n}(\gamma)$ is attainable at $\gamma = 0$. Numerical experiments suggest that the ratio α from the three largest eigenvalues of $B_{2n}(\gamma)$ is always bounded above. If this is true, then it would imply that the three

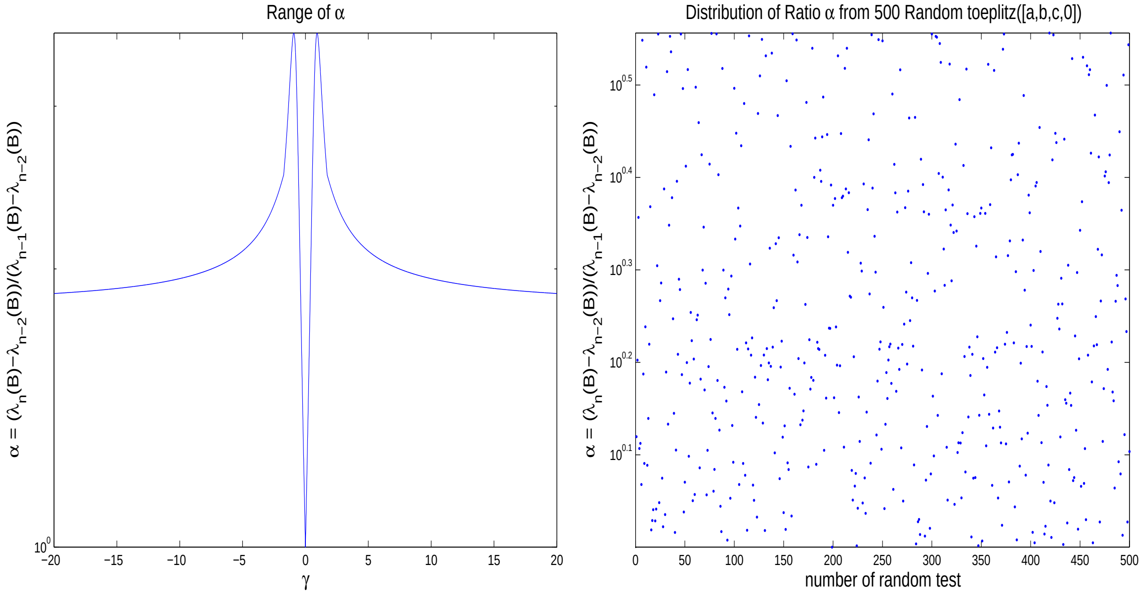

FIG. 3.2. *Attainable ratio α from γ and from 500 random tests.*

largest eigenvalues of pentadiagonal Toeplitz matrices cannot be arbitrarily assigned. In this section our goal is to prove the following theorem.

THEOREM 3.2. *Assume that n is even. The inverse problem of constructing a $n \times n$ symmetric pentadiagonal Toeplitz matrix with three given real numbers as its largest eigenvalues is not solvable if the ratio α determined by the three given numbers is too large.*

For convenience, denote the even dimensionality by $2n$. Let $P \in \mathbb{R}^{2n\times(2n-1)}$ be the matrix by deleting the last column of the identity matrix I_{2n}. Then $B_{2n-1} = P^\top B_{2n} P$. The interlacing between the largest few eigenvalues of $B_{2n-1}(\gamma)$ and $B_{2n}(\gamma)$ is stated as

$$\lambda_{2n-2}(B_{2n}) \leq \lambda_{2n-2}(B_{2n-1}) \leq \lambda_{2n-1}(B_{2n}) \leq \lambda_{2n-1}(B_{2n-1}) \leq \lambda_{2n}(B_{2n}). \tag{3.2}$$

Furthermore, observe that $X_{n-1} \mp \Xi_{n-1} Y_{n-1}$ are principal submatrices of $X_n \mp \Xi_n Y_n$, respectively. By the interlacing eigenvalues theorem for bordered matrices [8], the odd and even eigenvalues of $B_{2n}(\gamma)$ interlace with the odd and even eigenvalues of $B_{2(n-1)}(\gamma)$, respectively. Such a relationship between $B_4(\gamma)$ and $B_6(\gamma)$ is illustrated in Figure 3.3.

We have already proved in Theorem 2.6 that the largest eigenvalue of $B_n(\gamma)$ is simple, positive, and even for every n. We also know from Lemma 2.8 that the second largest eigenvalue of $B_n(\gamma)$ is always nonnegative, if $n \geq 4$. We now address the parity of $\lambda_{2n-1}(B_{2n})$.

LEMMA 3.3. *If $\gamma > 0$, then the second largest eigenvalue of $B_{2n}(\gamma)$ is odd unless it has multiplicity greater than one.*

Proof. We know that the even and odd eigenvalues of B_{2n} correspond to eigenvalues of $X_n + \Xi_n Y_n$ and $X_n - \Xi_n Y_n$, respectively. By Theorem 2.6, the largest eigenvalue of $B_{2n}(\gamma)$ is $\lambda_n(X_n + \Xi_n Y_n)$. So we only need to compare the second largest eigenvalue $\lambda_{n-1}(X_n + \Xi_n Y_n)$ of $X_n + \Xi_n Y_n$ with the

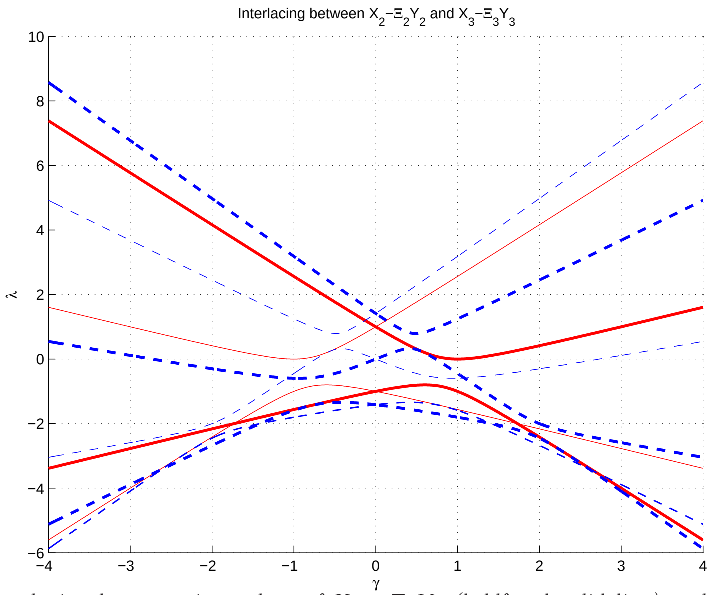

Fig. 3.3. *The interlacing between eigenvalues of $X_2 - \Xi_2 Y_2$ (boldfaced solid line) and $X_3 - \Xi_3 Y_3$ (boldfaced dashed line). The interlacing of even eigenvalues of $B_4(\gamma)$ and $B_6(\gamma)$ are mirror images drawn in thinner lines.*

largest eigenvalue $\lambda_n(X_n - \Xi_n Y_n)$ of $X_n - \Xi_n Y_n$. From (2.4), we see that

$$C := (X_n + \Xi_n Y_n) - (X_n - \Xi_n Y_n) = \begin{bmatrix} 0 & 0 & & & 0 \\ 0 & & & & \\ \vdots & & \ddots & & \\ 0 & 0 & & 0 & 2 \\ 0 & & & 2 & 2\gamma \end{bmatrix},$$

which has eigenvalues $\gamma - \sqrt{\gamma^2 + 4}, 0, \ldots, 0, \gamma + \sqrt{\gamma^2 + 4}$. By the Weyl theorem [8, Theorem 4.3.1], we know that

$$\lambda_{n-1}(X_n + \Xi_n Y_n) \leq \lambda_n(X_n - \Xi_n Y_n) + \lambda_{n-1}(C).$$

The second largest eigenvalue of $B_{2n}(\gamma)$ therefore is $\lambda_n(X_n - \Xi_n Y_n)$ because $\lambda_{n-1}(C) = 0$. ∎

We are now ready to prove the key result.

Theorem 3.4. *The second largest eigenvalue of $B_{2n}(\gamma)$ is always strictly greater than the second largest eigenvalue of $B_{2n-1}(\gamma)$, that is, $\lambda_{2n-2}(B_{2n-1}(\gamma)) < \lambda_{2n-1}(B_{2n}(\gamma))$ for all γ.*

Proof. We shall prove by contradiction. Assume at a certain $\gamma_0 > 0$,

$$\lambda_{2n-2}(B_{2n-1}(\gamma_0)) = \lambda_{2n-1}(B_{2n}(\gamma_0)) = \nu.$$

Denote orthonormal bases of eigenvectors of $B_{2n}(\gamma_0)$ and $B_{2n-1}(\gamma_0)$, respectively, by $\{\mathbf{u}_1, \ldots, \mathbf{u}_{2n}\}$ and $\{\mathbf{v}_1, \ldots, \mathbf{v}_\ell\}$. We may further assume, according to [3], that these eigenvectors are either even or odd. Let the invariant subspaces spanned by eigenvectors $\{\mathbf{u}_1, \ldots, \mathbf{u}_i\}$ and $\{\mathbf{v}_1, \ldots, \mathbf{v}_j\}$ be denoted by U_i and V_j, respectively. It follows that there exist a vector $\mathbf{y} \in \mathbb{R}^{2n-1}$ of B_{2n-1} from the subspaces

$$\mathbf{y} \in V_{2n-3}^{\perp} \bigcap (P^{\top} U_{2n-1}^{\perp})^{\perp},$$

such that

$$B_{2n-1}(\gamma_0)\mathbf{y} = \nu \mathbf{y},$$
$$B_{2n}(\gamma_0)\begin{bmatrix} \mathbf{y} \\ 0 \end{bmatrix} = \nu \begin{bmatrix} \mathbf{y} \\ 0 \end{bmatrix}.$$

By Theorem 2.6, the eigenvalue $\lambda_{2n-1}(B_{2n-1}(\gamma_0))$ is necessarily distinct from $\lambda_{2n-2}(B_{2n-1}(\gamma_0))$. The vector $\mathbf{y}$ therefore can only be in the space spanned by $\mathbf{v}_{2n-2}$ and, hence, $\mathbf{y}$ must be either even or odd.

If ν is simple, then by Lemma 3.3 the second eigenvector $[\mathbf{y}^\top, 0]^\top$ of B_{2n} must be an odd vector. If follows that $y_1 = 0$ and, hence, $\mathbf{y} = 0$. This contradicts with the fact that $\mathbf{y}$ is an eigenvector of B_{2n-1}. Thus ν must be a double eigenvalue. That is,

$$\lambda_{2n-2}(B_{2n}(\gamma_0)) = \lambda_{2n-2}(B_{2n-1}(\gamma_0)) = \lambda_{2n-1}(B_{2n}(\gamma_0)) = \nu.$$

By Theorem 2.10, the eigenvalue curves $\lambda_{2n-2}(B_{2n}(\gamma))$ and $\lambda_{2n-1}(B_{2n}(\gamma))$ must intersect transversally at γ_0. We know by Lemma 2.1 that the eigenvalue $\lambda_{2n-2}(B_{2n}(\gamma)$ is even for large enough γ. It thus follows that nearby γ_0 the parity of $\lambda_{2n-1}(B_{2n}(\gamma))$ must be changed. This contradicts with the result in Lemma 3.3. □

By Theorem 3.4, the second and the third eigenvalues of $B_{2n}(\gamma)$ are effectively separated according to (3.2). The following result together with the continuity and the asymptotic property of eigenvalue curves assert the statement made in Theorem 3.2.

Corollary 3.5. *There is always a gap between the second eigenvalue and the third eigenvalue of $B_{2n}(\gamma)$.*

We find it illuminating to demonstrate the interlacing relationship between eigenvalues of $B_4(\gamma)$, $B_5(\gamma)$, and $B_6(\gamma)$ in Figure 3.4. On the right margin we identify eigenvalue curves of $B_6(\gamma)$ by the

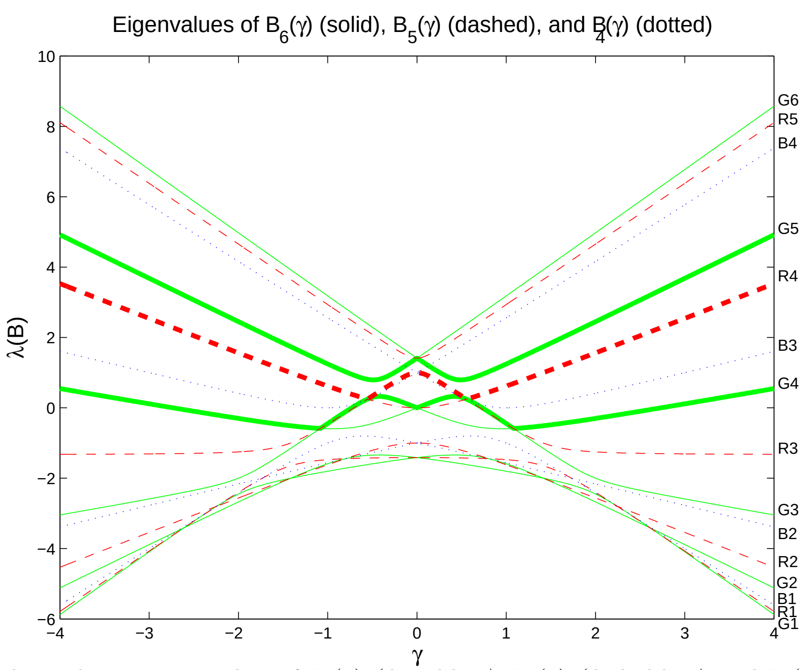

Fig. 3.4. *Interlacing between eigenvalues of $B_4(\gamma)$ (dotted line), $B_5(\gamma)$ (dashed line), and $B_6(\gamma)$ (solid line).*

prefixes "G" followed by its ordering. Similarly marked are the prefix "R" for the eigenvalues of

$B_5(\gamma)$ and "B" for $B_4(\gamma)$. Be aware of the gap between G5 and R4 as asserted by Theorem 3.4 and the separation of G5 and G4.

3.2. Odd Dimension. In contrast to the preceding discussion, our numerical experiments suggest that the ratio α from the three largest eigenvalues of $B_{2n-1}(\gamma)$ is always bounded away from 1 and has no upper bound. Our goal in this section is to establish the following result.

THEOREM 3.6. *Assume that n is odd. The inverse problem of constructing a $n \times n$ symmetric pentadiagonal Toeplitz matrix with three given real numbers as its largest eigenvalues is not solvable if the ratio α determined by the three given numbers is too close to 1.*

To establish Theorem 3.6, we first argue that the ratio α has no upper bound by showing that the denominator in (1.8) vanishes at some point. For convenience, we denote the odd dimensionality by $2n-1$.

THEOREM 3.7. *The curves of the second and the third largest eigenvalues of $B_{2n-1}(\gamma)$ must intersect at some $\gamma_0 > 0$.*

Proof. It is easy to check that the second largest eigenvalue of $B_{2n-1}(0)$ is given by

$$\lambda_{2n-2}(B_{2n-1}(0)) = 2\cos\frac{\pi}{n}$$

and has even parity. On the other hand, by Lemma 2.1, the eigenstructure of $B_{2n-1}(\gamma)$ behaves like that *toeplitz*$([0, 1, 0, \ldots, 0])$ when γ is sufficiently large. In particular, as γ goes to infinity, the second largest eigenvalue of $B_{2n-1}(\gamma)$ is asymptotically given by

$$\lim_{\gamma\to\infty} \frac{\lambda_{2n-2}(B_{2n-1}(\gamma))}{\gamma} = 2\cos\frac{\pi}{n}$$

which has odd parity. We have pointed out earlier in (2.7) the analyticity of eigenvalue curves. Consequently, each *ordered* eigenvalue curve must be at least continuous. The only possibility for the second largest eigenvalue curve to change its parity is at an intersection with the third largest eigenvalue curve which has the even parity at infinity. (See, for example, the eigenvalue curves R4 and R3 in Figure 3.4 for $B_5(\gamma)$.) ∎

The fact that the ratio α of the three largest eigenvalues of $B_{2n-1}(\gamma)$ is bounded away from 1 can be illustrated by the simple case $B_3(\gamma)$. It is not difficult to check that the ratio

$$\alpha = \frac{3 + \sqrt{1 + 8\gamma^2}}{3 - \sqrt{1 + 8\gamma^2}}$$

attains it minimal value $\alpha_{min} = 2$ at $\gamma = 0$. To see the general case, we write

$$\alpha = \frac{\lambda_{2n-1}(B_{2n-1}(\gamma)) - \lambda_{2n-3}(B_{2n-1}(\gamma))}{\lambda_{2n-2}(B_{2n-1}(\gamma)) - \lambda_{2n-3}(B_{2n-1}(\gamma))} = 1 + \frac{\lambda_{2n-1}(B_{2n-1}(\gamma)) - \lambda_{2n-2}(B_{2n-1}(\gamma))}{\lambda_{2n-2}(B_{2n-1}(\gamma)) - \lambda_{2n-3}(B_{2n-1}(\gamma))}. \tag{3.3}$$

By Lemma 2.1, we know that

$$\lim_{\gamma\to\infty} \frac{\lambda_{2n-1}(B_{2n-1}(\gamma)) - \lambda_{2n-2}(B_{2n-1}(\gamma))}{\lambda_{2n-2}(B_{2n-1}(\gamma)) - \lambda_{2n-3}(B_{2n-1}(\gamma))} = \frac{\cos\frac{\pi}{2n} - \cos\frac{2\pi}{2n}}{\cos\frac{2\pi}{2n} - \cos\frac{3\pi}{2n}} > 0.$$

Thus for γ large enough, there is a positive lower bound for the second term in (3.3). On the other hand, note that the difference $\lambda_{2n-1}(B_{2n-1}(\gamma)) - \lambda_{2n-2}(B_{2n-1}(\gamma))$ is never zero, because the largest eigenvalue $\lambda_{2n-1}(B_{2n-1}(\gamma)$ is always simple. By the continuity of the eigenvalue curves, over any fixed finite interval of γ there exist a positive minimal value, say δ_1, of $\lambda_{2n-1}(B_{2n-1}(\gamma)) - \lambda_{2n-2}(B_{2n-1}(\gamma))$ and positive maximal value, say δ_2, of $\lambda_{2n-2}(B_{2n-1}(\gamma)) - \lambda_{2n-3}(B_{2n-1}(\gamma))$. It follows that the second term in (3.3) is bounded away from $\frac{\delta_1}{\delta_2}$ over this finite interval. Together, there is a positive lower bound for the second term in (3.3) over the interval $[0, \infty)$.

LEMMA 3.8. *For each given n, there exists a positive number δ such that ratio from the three largest eigenvalues of $B_{2n-1}(\gamma)$ is at least $1+\delta$ for all γ.*

We conjecture that the minimal ratio α_{min} occurs at $\gamma = 0$ with the value

$$\alpha_{min} = \frac{\cos\frac{\pi}{n+1} - \cos\frac{2\pi}{n+1}}{\cos\frac{\pi}{n} - \cos\frac{2\pi}{n+1}}$$

which converges to 1 as n goes to infinity. We do not have a proof of the conjecture yet, but Theorem 3.7 and Lemma 3.8 are sufficient to establish Theorem 3.6.

4. Computation. In the preceding section, our emphasis has been on the theoretical issue of solvability. In particular, we have shown that the three largest eigenvalues of symmetric pentadiagonal Toeplitz matrix cannot be arbitrarily assigned. More specifically, if n is even and if the ratio α is too large, or if n is odd and if the ratio α is too close to 1, then inverse eigenvalue problem is not solvable. In this section, we describe how the solution, if exists, can be found numerically by using the recursive formula (2.3).

The basic idea is to apply the Newton method to iterate on the parameters a, b, and c. That is, given three values $\lambda_i < \lambda_j < \lambda_k$ whose ratio α is known a priori to be in the range of R_{ijk}, we solve the system of equations,

$$f(a,b,c) := \begin{bmatrix} \rho_n(\lambda_i; a,b,c) \\ \rho_n(\lambda_j; a,b,c) \\ \rho_n(\lambda_k; a,b,c) \end{bmatrix} = 0, \tag{4.1}$$

by the standard scheme

$$\begin{bmatrix} a^{(\ell+1)} \\ b^{(\ell+1)} \\ c^{(\ell+1)} \end{bmatrix} = \begin{bmatrix} a^{(\ell)} \\ b^{(\ell)} \\ c^{(\ell)} \end{bmatrix} - \begin{bmatrix} \nabla^\top \rho_n(\lambda_i; a^{(\ell)}, b^{(\ell)}, c^{(\ell)}) \\ \nabla^\top \rho_n(\lambda_j; a^{(\ell)}, b^{(\ell)}, c^{(\ell)}) \\ \nabla^\top \rho_n(\lambda_k; a^{(\ell)}, b^{(\ell)}, c^{(\ell)}) \end{bmatrix}^{-1} f(a^{(\ell)}, b^{(\ell)}, c^{(\ell)}). \tag{4.2}$$

The derivative information can be obtained effectively from the following recursive algorithm.

ALGORITHM 4.1. *Given a value λ, the evaluation of $\rho_n(\lambda; a,b,c)$ and its gradient with respect to the three parameters (a,b,c) can be obtained from the following recursive formula:*

1. *Define the 4×5 matrix Φ by*

$$\Phi := \begin{bmatrix} c^5 & c^4 - (a-\lambda)c^3 & b^2c - (a-\lambda)c^2 & (a-\lambda)c - b^2 & (a-\lambda) - c \\ 0 & -c^3 & -c^2 & c & 1 \\ 0 & 0 & 2bc & -2b & 0 \\ 5c^4 & 4c^3 - 3(a-\lambda)c^2 & b^2 - 2c(a-\lambda) & (a-\lambda) & -1 \end{bmatrix}.$$

2. *Initiate the 4×5 matrix Ψ by defining*

$$\Psi := \begin{bmatrix} 0 & 1 & (a-\lambda) & (a-\lambda)^2 - b^2 & (a-\lambda)^3 - (a-\lambda)(2b^2+c^2) + 2cb^2 \\ 0 & 0 & 1 & 2(a-\lambda) & 3(a-\lambda)^2 - (2b^2+c^2) \\ 0 & 0 & 0 & -2b & -4(a-\lambda)b + 4bc \\ 0 & 0 & 0 & 0 & -2(a-\lambda)c + 2b^2 \end{bmatrix}.$$

3. *Repeat the following process $n-3$ times.*
   (a) *Compute the 4×1 vector*

$$\mathbf{u} := \Phi(1,:)\Psi^\top + \Psi(1,:)\Phi^\top.$$

n	3	4	5	6	7	8	9	10	11	12
a	6.6667	5.2882	3.7546	2.1118	0.4342	-1.1864	-2.6445	-3.8231	-4.5979	-4.8510
b	1.7638	2.4237	3.1520	3.9107	4.6446	5.2893	5.7715	6.0107	5.9212	5.4209
c	-0.3333	-0.2370	-0.1842	-0.1172	-0.0110	0.1551	0.4020	0.7521	1.2289	1.8557

n	13	14	15	16	17	18	19	20	21	22
a	-4.5142	-3.7345	-3.2927	-3.7167	-4.9640	-6.0918	-7.5683	-8.9302	-10.5078	-12.0385
b	4.4599	3.1353	1.9940	1.4224	1.4181	1.2690	1.3386	1.2656	1.3099	1.2630
c	2.6482	3.5828	4.5026	5.2854	5.9116	6.6236	7.2908	8.0439	8.7873	9.5988

n	23	24	25	26	27	28	29	30	31	32
a	-13.7343	-15.4168	-17.2375	-19.0650	-21.0142	-22.9833	-25.0629	-27.1718	-29.3829	-31.6303
b	1.2949	1.2611	1.2855	1.2595	1.2791	1.2583	1.2744	1.2572	1.2709	1.2564
c	10.4141	11.2886	12.1739	13.1132	14.0676	15.0727	16.0959	17.1672	18.2588	19.3967

TABLE 4.1
Pentadiagonal Toeplitz matrices of size $n = 3, \ldots, 32$ with dominant eigenvalues $\{4, 7, 9\}$.

(b) Update the matrix Ψ by defining

$$\Psi := \begin{bmatrix} & \frac{u_1}{2} \\ \Psi(:,2:5) & u_2 \\ & u_3 \\ & u_4 \end{bmatrix}.$$

4. Retrieve the values

$$\rho_n(\lambda; a, b, c) = \Psi(1, 5),$$
$$\nabla\rho_n(\lambda; a, b, c) = \Psi(2:4, 5).$$

It should be noted that upon convergence, the limit point of the iteration will satisfy the equation (4.1). Such a bearing, however, only guarantees that the triplet $\{\lambda_i, \lambda_j, \lambda_k\}$ is a portion in the spectrum of the corresponding *toeplitz*$([a, b, c, 0, \ldots])$. It does not secure that each of the given eigenvalues, say, λ_k, maintains its order, say, the k-th largest, in the spectrum. Clearly, in order to keep the given order, the initial value for the iteration scheme must be carefully selected. An interesting discussion about the importance of initial approximation to the full *regular* Toeplitz matrix considered by Landau [10] can be found in [11].

We are particularly interested in constructing a pentadiagonal Toeplitz matrix with three prescribed largest eigenvalues $\lambda_{n-2} \leq \lambda_{n-1} \leq \lambda_n$. In our experiments, we choose to start with the tridiagonal Toeplitz matrix *toeplitz*$([a_0, b_0, 0, \ldots])$ whose first two largest eigenvalues are λ_{n-1} and λ_n (See (1.1)). It appears that whenever there exists a solution, the iteration from this initial value always converges satisfactorily. We still do not fully understand the reason yet.

We present one numerical example. Suppose $\{4, 7, 9\}$ are the desirable three largest eigenvalues with the ratio $\alpha = \frac{5}{3}$. Presented in Table 4.1 are the values of a, b, c (up to four decimal digits) in the pentadiagonal Toeplitz matrices *toeplitz*$([a, b, c, 0, \ldots])$ of sizes $n = 3, \ldots 32$. It turns out all these 30 matrices in this table have the same $\{4, 7, 9\}$ as their largest three eigenvalues.

5. Conclusion and Future Work. For the pentadiagonal Toeplitz matrices, we have discovered a surprising but interesting result. The difference quotient α of the largest three eigenvalues, defined by (1.8), plays a critical role. When n is even, this ratio can be as small as one, but cannot be too large. When n is odd, this ratio can be arbitrarily large, but cannot be too close to one. This necessary and sufficient condition is innovative. It also provides a theoretical ground to answer the inverse eigenvalue problem under the pentadiagonal Toeplitz structure. A Newton-type iterative method can be employed to construct such a matrix numerically.

What has not been studied in this paper is to derive the threshold of α above which or below which the inverse eigenvalue problem is not solvable. In view of the example demonstrated in Table 4.1, it would be interesting to see whether a least upper bound or a greatest lower bound exists and is independent of the size n. It would be of practical importance to justify why our proposed tridiagonal initial value always works.

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