Electronic Transactions on Numerical Analysis.
Volume 58, pp. 316–347, 2023.

ISSN 1068–9613.
DOI: 10.1553/etna_vol58s316

ETNA
Kent State University and
Johann Radon Institute (RICAM)

IMPROVED BISECTION EIGENVALUE METHOD FOR BAND SYMMETRIC TOEPLITZ MATRICES*

YULI EIDELMAN† AND IULIAN HAIMOVICI†

Abstract. We apply a general bisection eigenvalue algorithm, developed for Hermitian matrices with quasiseparable representations, to the particular case of real band symmetric Toeplitz matrices. We show that every band symmetric Toeplitz matrix T_q with bandwidth q admits the representation $T_q = A_q + H_q$, where the eigendata of A_q are obtained explicitly and the matrix H_q has nonzero entries only in two diagonal blocks of size $(q-1) \times (q-1)$. Based on this representation, one obtains an interlacing property of the eigenvalues of the matrix T_q and the known eigenvalues of the matrix A_q. This allows us to essentially improve the performance of the bisection eigenvalue algorithm. We also present an algorithm to compute the corresponding eigenvectors.

Key words. Toeplitz, quasiseparable, banded matrices, eigenstructure, inequalities, Sturm with bisection

AMS subject classifications. 15A18, 65F15, 65F50, 15A42, 65N25

1. Introduction. We study the problem of computing a part or all of the set of eigenvalues of band symmetric Toeplitz matrices. We use an approximation of Toeplitz matrices by matrices from a special class, for which we compute the eigenvalues explicitly. Given an $N \times N$ q-band symmetric Toeplitz matrix T_q with the only nonzero entries

$$T_q(i,j) = t_{|i-j|}, \qquad |i-j| \leq q, \quad i,j = 1,\dots,N,$$

we define the matrix A_q via perturbations of the matrix T_q at the left-top and the right-bottom corners. Namely, we set for the perturbed matrix A_q

$$A_q(i,j) = t_{|i-j|} - t_{i+j}, \qquad \text{for } i+j \leq q \text{ and for } 2N-q+2 \leq i+j \tag{1.1}$$

and $A_q(i,j) = T_q(i,j)$ otherwise. In particular, if $|i-j| > q$, then $A_q(i,j) = 0$. So we get $T_q = A_q + H_q$, where the matrix H_q has nonzero entries only in two extreme diagonal blocks of size $(q-1) \times (q-1)$, and this is independent of the size N. For instance,

$$A_4(1:5,1:5) = \begin{bmatrix} t_0 - t_2 & t_1 - t_3 & t_2 - t_4 & t_3 & t_4 \\ t_1 - t_3 & t_0 - t_4 & t_1 & t_2 & \ddots \\ t_2 - t_4 & t_1 & t_0 & \ddots & \ddots \\ t_3 & t_2 & \ddots & \ddots & \\ t_4 & \ddots & \ddots & & \end{bmatrix}. \tag{1.2}$$

This kind of matrices have also been used in [2], not as a perturbation of an $N \times N$ Toeplitz matrix, but because they embed as a submatrix a smaller-sized Toeplitz matrix. For instance, the $N \times N$ matrix A_4 from (1.2) embeds the $(N-4) \times (N-4)$ Toeplitz matrix $T = A_4(3:N-2, 3:N-2)$. However, the results that we obtain use A_q as a small-rank perturbation of a Toeplitz matrix T_q of the same size $N \times N$ as A_q.

*Received May 30, 2019. Accepted January 16, 2023. Published online on March 30, 2023. Recommended by Michiel Hochstenbach.
†School of Mathematical Sciences, Raymond and Beverly Sackler Faculty of Exact Sciences, Tel-Aviv University, Ramat-Aviv 69978, Israel (eideyu@post.tau.ac.il, iulianh@zahav.net.il).

We found that if $t_q > 0$, which we can presume without loss of generality, then the eigenvalues of the such obtained matrix A_q, for any N, are

$$t_0 + 2\sum_{j=1}^{q} t_j \cos\left(\frac{jk\pi}{N+1}\right), \qquad k = 1, \ldots, N. \tag{1.3}$$

Moreover, we also prove that this set may be sorted in ascending order to almost interlace with the eigenvalues of T_q (see for instance (1.5) below).

More precisely, we denote the nondecreasing eigenvalues of A_q and of T_q, for $k = 1, \ldots, N$, by λ_k^A and λ_k^T, respectively, and we suppose that the corner matrix

$$H_q(1:q-1, 1:q-1) = T_q(1:q-1, 1:q-1) - A_q(1:q-1, 1:q-1)$$

is strongly regular (i.e., all its principal leading submatrices $H_q(1:m, 1:m)$, for the indices $m = 1, \ldots, q-1$, are regular). By the interlacing property we mean that if we denote by n the number of negative eigenvalues of H_q and by $p = q - 1 - n$ the number of its positive eigenvalues (including multiplicities), then

$$\lambda_{k-2n}^A \le \lambda_k^T \le \lambda_{k+2p}^A, \qquad k = 2n+1, \ldots, N-2p. \tag{1.4}$$

From (1.4) it follows that for $q = 2$ (pentadiagonal matrices), the eigenvalues of A_2 and T_2, except of the two last ones, interlace; more precisely,

$$\lambda_k^A \le \lambda_k^T \le \lambda_{k+2}^A, \qquad k = 1, \ldots, N-2. \tag{1.5}$$

For 3-band (heptadiagonal) matrices, i.e., $q = 3$, we obtain that the eigenvalues of A_3 and T_3 satisfy (1.4) with $p = n = 1$. Using the form of the perturbing matrix H_q, we apply known results about small symmetric matrix perturbations of a symmetric matrix in order to approximate the eigenvalues of T_q. For instance, we show in (4.4) that if m_k, $k = 1, \ldots, N$, are the unwanted differences between the eigenvalues of T_q and A_q, then $\sum_{k=1}^{N} m_k^2 \le 2\sum_{j=1}^{q-1} j t_{j+1}^2$, and this is independent of the size N of the matrices T_q and A_q. The approximation is better for larger matrices and/or tridiagonally dominated matrices (which, for instance, can mean that $|t_1| \ge \sum_{j=2}^{q} |t_j|$). We verified this for 5-band 10000×10000 matrices with $t_j = t_0/2^j$, $j = 1, \ldots, 5$, and we obtained five exact digits. This permits us to find lower and upper bounds when we look only for selected eigenvalues of T_q.

As stated above, we study a fast algorithm for the numerical solution of the eigenvalue problem for band symmetric Toeplitz matrices. We obtain the solution of the problem using quasiseparable representations of the considered matrices. Quasiseparable representations as a tool to design various fast matrix algorithms have been introduced in [6], their eigenstructure was first treated in [9], and they were extensively studied in the monograph [7, 8].

In Section 5 we present some basic information on this subject, and we easily obtain the quasiseparable representation (quasiseparable generators) for q-band symmetric Toeplitz matrices. To solve the eigenproblem, we apply the bisection algorithm developed for quasiseparable Hermitian matrices in [11] to the particular case of band symmetric Toeplitz matrices. The interlacing properties between the eigenvalues of T_q and the in advance known eigenvalues of A_q mentioned above allow us to essentially improve the performance of the bisection eigenvalue algorithm. The performance of the algorithm is illustrated by numerical tests. We also derive an algorithm to compute the eigenvectors. Usually, for other types of matrices, our algorithm for finding eigenvectors is unstable since it performs many multiplications with complex numbers and it requires additional work in the future to improve its accuracy. However, the results of the numerical tests show that, for the considered class of band symmetric

Toeplitz matrices, this algorithm works very well even for huge matrices, as Figures 6.2–6.4 illustrate.

Since the formulas for the eigenvalues (2.2) and eigenvectors (2.4) of tridiagonal Toeplitz matrices are known, many authors gave special attention to the next smaller case, that of pentadiagonal matrices. Appendix A is devoted to them, where a special and much faster complete algorithm is devised. We use, for instance, the fact that these matrices do not have multiple eigenvalues. We also show that in many cases the eigenvalues of the perturbed matrices are already monotonous, which means that in (1.3), the eigenvalues are decreasing or increasing in k without the need to sort them any more (e.g., if $|t_1| \geq 4t_2$). (Extensive numerical experiments suggest that in these cases and for even k, we have $\lambda_k^A \leq \lambda_k^T \leq \lambda_{k+1}^A$, but we do not claim this since we did not yet prove it. We would like to conjecture this interlacing property.)

The eigenvalue problem for band symmetric Toeplitz matrices has been studied by other authors. The closest work to our paper is that by Bini and Capovani [2]. In [2] the authors also used the matrices A_q defined above. They reach those for other reason, i.e., through the fact that they embed an $N \times N$ band symmetric Toeplitz matrix as their submatrix. For 2- and 3-band matrices, one obtains $(N+2) \times (N+2)$ matrices A_q and nicer results for the eigenstructure of the core $N \times N$ Toeplitz matrices which they surround. For the 4- and 5-band case, an $(N+4) \times (N+4)$ embedding matrix is needed, and the size grows with the size of the band.

In the paper [12] the formulas (1.3) are used in order to asymptotically approximate the eigenvalues of T_q, but they are not linked there to the matrix A_q or to the inequalities (1.4).

The motivation of the present paper is as follows. We have previously published the article [11] on a bisection algorithm for general Hermitian matrices given in quasiseparable form. Numerical experiments showed that for large matrices (up to 32768×32768) with complex entries and with a high order of quasiseparability, the error was much larger than for quasiseparable Hermitian matrices of order one (for which we published a simpler algorithm [10]). For eigenvectors of matrices with higher order of quasiseparability, the orthogonality was lost even for 128×128 matrices. But this does not happen for band symmetric Toeplitz matrices, and we will now explain why.

Since our algorithms repeatedly multiply matrices with the quasiseparable generators, which are small matrices, we decided to investigate symmetric q-band matrices, which are an example of quasiseparable matrices of order q and their quasiseparable generators contain, as usual, $q(q+2)$ entries all in all, where q^2 entries are zero, q entries are equal to 1, and q entries are real numbers.

While treating $N \times N$ band symmetric Toeplitz matrices, since the eigenvectors of all the tridiagonal ones are the same, we decided to multiply them and to add at each step scalar matrices (by this we mean matrices sI_N, where s is a real number and I_N is the identity matrix). The resulting matrices would all have the same eigenvectors so that the eigenvalues can be computed by multiplications and additions. We soon recognized that the same class of matrices, with each member being a perturbation of a certain Toeplitz matrix, can entirely be obtained by multiplying all the time only with the T_M matrix from (2.1).

When searching the papers in this field, we found that results closest to ours are contained in the work of Bini and Capovani [2] and also, briefly, in the book [4]. However, we were delighted to see that none of their results and none of their proofs resemble ours. First of all, they do not mention fast bisection algorithms by using the quasiseparable generators, while we do not replicate any results that are similar to theirs (for instance, those on their last 7 pages). They reach the same class of matrices, but, while we use an $N \times N$ perturbation matrix of an $N \times N$ Toeplitz matrix, they employ a larger matrix since such an $(N + 2\lfloor q/2 \rfloor) \times (N + 2\lfloor q/2 \rfloor)$

ETNA
Kent State University and
Johann Radon Institute (RICAM)

matrix embeds an $N \times N$ q-band symmetric Toeplitz matrix, where $\lfloor z \rfloor$ stands for the largest integer which is less than or equal to the real number z.

In their Table 1, the core matrix of the 14×14 matrix is the 8×8 Toeplitz matrix with Toeplitz coefficients a_1 to a_7 (where i stands in the table for a_i, and these coefficients would be denoted in our paper as $t_0, \ldots, t_6$). In our paper, such a matrix would correspond here to a 14×14 Toeplitz matrix.

There are only 3 formulas that both us and them tried to find:

1. **The formula for the eigenvalues of the perturbing class of matrices**, for which we find a closed formula (1.3) for any N and any bandwidth in Section 3, while they do not present this nice formula (see Proposition 2.2 and Remark 1 in [2]).
2. **The bounds for the Toeplitz eigenvalues of a 3-band matrix with even size N**, which are interesting only since they devote to this case a large portion of their paper and only after that, they extrapolate part of the results to the general band case. For such matrices, we obtain bounds as a particular case by substituting $q = 3$ in the set (1.3) after an ordering in nondecreasing order. We denote them as

$$\lambda_k^A = t_0 + 2\sum_{j=1}^{3} t_j \cos\left(\frac{jk\pi}{N+1}\right),$$

and then we obtain in Section 4 the following bounds for the nondecreasing eigenvalues of the 3-band symmetric Toeplitz matrix:

$$\lambda_{r-2}^A \le \lambda_r^T \le \lambda_{r+2}^A,$$

where $3 \le r \le N-2$ and λ_r^T, λ_r^A are the rth eigenvalue in the nondecreasing set of eigenvalues of the specified matrix. See [2, Section 3] for their result.
3. **The bounds for the Toeplitz eigenvalues of a q-band matrix**. Our interlacing property, as we prove it in Section 4, is completely different than that of the mentioned article, and with the same proof it is true for any two Hermitian matrices which differ by diagonal blocks.

Other related papers. In [14, 21], bisection is used to find the eigenvalues of a 2-band symmetric Toeplitz matrix. In the paper [13] the approximation of the eigenvalues of a band symmetric Toeplitz matrix by the values of its symbol on a special grid has been considered. See also [22] by Serra Capizzano and Sesana, and [3] by Bini and Pan.

The present paper contains seven sections and an appendix. Section 1 is the introduction. In Section 2 we treat the band symmetric Toeplitz matrices as a class of perturbations of matrices for which the spectra is obtained explicitly. In Section 3 we derive the formulas (1.3) for the eigenvalues of these perturbed matrices. In Section 4 we obtain the overall bounds and the interlacing properties for eigenvalues of band symmetric Toeplitz matrices and their perturbed matrices. In Section 5 we present the basics of quasiseparable representations of matrices, and we obtain a fast bisection eigenvalue algorithm by using quasiseparable generators of band Toeplitz matrices for finding (clusters of selected) eigenvalues. In Section 6 we illustrate our algorithms by numerical tests. Section 7 is the conclusion. In Appendix A we consider the particular case of 2-band matrices, for which better information on the location of the spectrum is obtained and the algorithm can be further improved.

2. Properties of the classes of matrices.

At first, consider the set of all tridiagonal $N \times N$ symmetric Toeplitz matrices. Out of such matrices, we will frequently use the one that has all its nonzero entries equal to 1 since it is convenient to multiply with it. It will be further denoted by T_M, i.e.,

$$T_M = \begin{bmatrix} 1 & 1 & 0 & \dots & & \\ 1 & 1 & 1 & 0 & \dots & \\ 0 & 1 & 1 & 1 & & \\ & & \ddots & \ddots & & \\ & & 0 & 1 & 1 & \end{bmatrix}. \tag{2.1}$$

As it is well known (see for instance [19] or [23, p. 212]) the eigenvalues of a tridiagonal Hermitian Toeplitz matrix (not necessarily a real symmetric one) with the entry t_0 on its main diagonal and the entry t_1 on its two sub-diagonals, are known to be

$$\lambda_k = t_0 + 2\,|t_1| \cos\left(\frac{k\pi}{N+1}\right), \quad k = 1, \dots, N. \tag{2.2}$$

In particular, the eigenvalues of T_M are

$$\lambda_k^{(M)} = 1 + 2\ \cos\left(\frac{k\pi}{N+1}\right), \quad k = 1, \dots, N. \tag{2.3}$$

Moreover, the eigenvectors of a tridiagonal Hermitian Toeplitz matrix are dependent only upon the argument of the (possibly complex) number t_1 and not on its absolute value or on t_0. It follows that all the real tridiagonal symmetric Toeplitz matrices share the same eigenvectors. Indeed, if on the first subdiagonal of a matrix T_1 the value t_1 is positive, then its argument is always 0, and if, on the contrary, $t_1 < 0$, then we also change the sign of t_0 and we obtain that our matrix is in fact $-T_1 + 2t_0 I_N$, which has the same eigenvectors as T_1. In the remaining case, when $t_1 = 0$, the matrix T_1 is not even tridiagonal, but it is the scalar matrix $t_0 I_N$.

In normalized form, these eigenvectors are

$$x_k(j) = \sqrt{\frac{2}{N+1}} \sin\left(\frac{kj\pi}{N+1}\right), \quad k, j = 1, \dots, N, \tag{2.4}$$

but this result, cited also in [2], will not be further used by us.

Since the eigenvectors are the same, the eigenvalues of products of such matrices, plus scalar multiples of the identity matrix, can be easily computed, so that we tried to see which matrices can be obtained in this way. The resulting class of matrices is what we call in this paper perturbations of band symmetric Toeplitz matrices, and we concluded that the whole class is obtained even if we use only repeated multiplications of a certain tridiagonal matrix T_1 with T_M from (2.1). It is convenient to multiply with a matrix which has all its nonzero entries equal to 1.

For a given tridiagonal symmetric Toeplitz matrix T_1 and a given sequence of real numbers δ_k, $k = 2, 3, \dots$, we define the sequence of matrices A_j, $j = 1, 2, \dots$, via recursive relations

$$A_1 = T_1, \quad A_j = A_{j-1} T_M + \delta_j I_N, \qquad j = 2, 3, \dots$$

Any such obtained matrix is in fact, as we will see, a perturbation (1.1) of a T_k, $k \geq 2$, matrix. For a given k-band symmetric Toeplitz matrix T_k with the only nonzero entries $T_k(i,j) = t_{|i-j|}$, $|i-j| \leq k$, we define the perturbation A_k via

$$A_k(i,j) = t_{|i-j|} - t_{i+j}, \qquad i + j \leq k, \tag{2.5}$$

$$A_k(i,j) = T_k(i,j), \qquad k < i + j < 2N - k + 2, \tag{2.6}$$

$$A_k(i,j) = t_{|i-j|} - t_{2N+2-i-j}, \qquad 2N - k + 2 \leq i + j. \tag{2.7}$$

ETNA
Kent State University and
Johann Radon Institute (RICAM)

The next theorem finds for a given band symmetric Toeplitz matrix T_q the corresponding T_1 and the scalars δ_j, $j = 2, \ldots, q$. Note that T_q can be completely described by its $q+1$ Toeplitz coefficients, and we will find another set of $q+1$ real numbers, $t_0^{(1)}, t_1^{(1)}, \delta_j$, $j = 2, \ldots, q$, to parameterize it.

THEOREM 2.1. *Consider a given* q*-band symmetric Toeplitz matrix* T_q *with the only nonzero entries* $T_q(i,j) = t^{(q)}_{|i-j|}$, $|i-j| \le q$. *Define the sequence* T_m, $m = q, q-1, \ldots, 1$, *of* m*-band symmetric Toeplitz matrices* T_m *with the only nonzero entries* $T_m(i,j) = t^{(m)}_{|i-j|}$, *with* $|i-j| \le m$, *satisfying for* $m = q, \ldots, 3, 2$ *the backward recursive relation*

$$t_j^{(m-1)} = \sum_{p=0}^{\lfloor \frac{m-j-1}{3} \rfloor} t^{(m)}_{j+1+3p} - \sum_{p=0}^{\lfloor \frac{m-j-2}{3} \rfloor} t^{(m)}_{j+2+3p}, \qquad j = 0, \ldots, m-1. \tag{2.8}$$

Here $\lfloor z \rfloor$ *denotes the largest integer less than or equal to the real number* z.

Then the corresponding perturbed matrices A_k, $k = 1, \ldots, q$, *satisfy the recursive relations*

$$A_1 = T_1, \quad A_k = A_{k-1} T_M + \delta_k I_N, \qquad k = 2, 3, \ldots, q, \tag{2.9}$$

with the coefficients δ_k *defined by the formulas*

$$\delta_k = t_0^{(k)} - 2t_1^{(k-1)} - t_0^{(k-1)}, \qquad k = 2, \ldots, q. \tag{2.10}$$

Proof. The proof is done by induction on k. Using (2.8) with $k = 2$ and $j = 0, 1$, we get

$$t_0^{(1)} = t_1^{(2)} - t_2^{(2)}, \qquad t_1^{(1)} = t_2^{(2)}. \tag{2.11}$$

Using (2.10) with $k = 2$, we get

$$\delta_2 = t_0^{(2)} - 2t_1^{(1)} - t_0^{(1)} = t_0^{(2)} - t_1^{(2)} - t_2^{(2)}. \tag{2.12}$$

Next using (2.5), (2.6), (2.7) with $k = 2$ we have

$$A_2(1,1) = t_0^{(2)} - t_2^{(2)} = A_2(N,N), \quad A_2(i,j) = T_2(i,j), \qquad 1 \le i+j \le N-1,$$

which because of (2.11), (2.12) imply

$$\begin{aligned}
A_2(1,1) = A_2(N,N) &= 2t_1^{(1)} + t_0^{(1)} - t_1^{(1)} = t_1^{(1)} + t_0^{(1)}, \\
A_2(i+1,i) = A_2(i,i+1) &= t_1^{(1)} + t_0^{(1)}, && i = 1, \ldots, N-1, \\
A_2(i+2,i) = A_2(i,i+2) &= t_1^{(1)}, && i = 1, \ldots, N-2, \\
A_2(i,j) &= 0, && |i-j| > 2.
\end{aligned} \tag{2.13}$$

Next using (2.1) we obtain directly that

$$A_1 T_M = T_1 T_M = \begin{bmatrix}
t_0+t_1 & t_0+t_1 & t_1 & & \cdots & \\
t_0+t_1 & t_0+2t_1 & t_0+t_1 & t_1 & \cdots & \\
t_1 & t_0+t_1 & t_0+2t_1 & t_0+t_1 & \ddots & \vdots \\
 & t_1 & t_0+t_1 & t_0+2t_1 & \ddots & \\
 & & t_1 & t_0+t_1 & \ddots & \\
 & & & & \ddots & \\
 & & \cdots & & & t_0+t_1
\end{bmatrix},$$

ETNA
Kent State University and
Johann Radon Institute (RICAM)

where t_0, t_1 are in fact $t_0^{(1)}, t_1^{(1)}$, respectively. Hence using (2.11), (2.12) and comparing with (2.13), we conclude that $A_2 = A_1 T_M + \delta_2 I_N$.

Now assume that a set T_k, $k = 1, 2, \dots, q-1$, of k-band symmetric Toeplitz matrices with the only nonzero entries $T_k(i,j) = t_{|i-j|}^{(k)}$, $|i-j| \le k$, satisfy (2.8). By the definitions (2.5)–(2.7), we have

$$A_q(i,j) = t_{|i-j|}^{(q)} - t_{i+j}^{(q)}, \qquad i+j \le q, \tag{2.14}$$

$$A_q(i,j) = T_q(i,j), \qquad q < i+j < 2N-q+2 \tag{2.15}$$
$$A_q(i,j) = t_{|i-j|}^{(q)} - t_{2N-i-j+2}^{(q)}, \qquad 2N-q+2 \le i+j.$$

Consider the matrix $B_q = A_{q-1} T_M + \delta_q I_N$. Using the formula (2.1) we have

$$B_q(i,j) = A_{q-1}(i,j-1) + A_{q-1}(i,j) + A_{q-1}(i,j+1) + \delta_q \delta_{ij}, \qquad 1 \le i,j \le N \tag{2.16}$$

(with $A_{q-1}(i,0) = A_{q-1}(i,N+1) = 0$). To compare the matrices A_q and B_q, consider the subdiagonal parts of the ith row, $i = q+1, \dots, 2N-q$, of the matrix A_q. Using (2.15) we have

$$A_q(i, 1:i-1) = T_q(i, 1:i-1) = \begin{bmatrix} 0_{1\times(i-q-1)} & t_q^{(q)} & t_{q-1}^{(q)} & \dots & t_1^{(q)} \end{bmatrix}. \tag{2.17}$$

Using (2.15) with $q-1$ instead of q we have

$$A_{q-1}(i, 1:i) = \begin{bmatrix} 0_{1\times(i-q-1)} & 0 & t_{q-1}^{(q-1)} & t_{q-2}^{(q-1)} & \dots & t_1^{(q-1)} & t_0^{(q-1)} \end{bmatrix},$$
$$i = q+1, \dots, 2N-q.$$

Using (2.16) we obtain

$$B_q(i, 1:i-1)$$
$$= \begin{bmatrix} 0 & t_n^{(n)} & t_n^{(n)} + t_{q-2}^{(n)} & t_n^{(n)} + t_{q-2}^{(n)} + t_{q-3}^{(n)} & \dots & t_3^{(n)} + t_2^{(n)} + t_0^{(n)} \end{bmatrix}, \tag{2.18}$$
$$i = q+1, \dots, N-q,$$

where $n = q-1$ and the leading 0 is of size $0_{1\times(i-q-1)}$. Thus, the relations (2.17) and (2.18) imply that the identities

$$A_q(i, 1:i-1) = B_q(i, 1:i-1), \qquad i = q+1, \dots, 2N-q \tag{2.19}$$

are equivalent to the linear upper triangular system of q equations

$$t_{q-1}^{(q-1)} = t_q^{(q)},$$
$$t_{q-1}^{(q-1)} + t_{q-2}^{(q-1)} = t_{q-1}^{(q)}, \tag{2.20}$$
$$t_{j+1}^{(q-1)} + t_j^{(q-1)} + t_{j-1}^{(q-1)} = t_j^{(q)}, \qquad j = q-2, \dots 1,$$

with a nonsingular matrix. The formulas (2.8) yield the solution of this system. Hence, equality (2.19) follows.

Next consider the diagonal entries $A_q(i,i)$ and $B_q(i,i)$ with $i = q+1, \dots, N-q$. Using (2.15) we have $A_q(i,i) = t_0^{(q)}$. Using (2.16) with $i = j$, we get

$$B_q(i,i) = t_1^{(q-1)} + t_0^{(q-1)} + t_1^{(q-1)} + \delta_q,$$

ETNA
Kent State University and
Johann Radon Institute (RICAM)

which, because of (2.10), means that $B_q(i,i) = t_0^{(q)}$, i.e., $A_q(i,i) = B_q(i,i)$. The latter together with (2.19) means

$$A_q(i, 1:i) = B_q(i, 1:i), \qquad i = q+1, \dots, 2N-q.$$

Next for $i = 1, 2, \dots, \lfloor q/2 \rfloor$, using (2.14), we obtain

$$A_q(i, 1:i-1) = \begin{bmatrix} t_{i-1}^{(q)} - t_{i+1}^{(q)} & t_{i-2}^{(q)} - t_{i+2}^{(q)} & \dots & t_1^{(q)} - t_{2i-1}^{(q)} \end{bmatrix}.$$

The corresponding subrow in the matrix A_{q-1} is

$$A_{q-1}(i, 1:i) = \begin{bmatrix} t_{i-1} - t_{i+1} & t_{i-2} - t_{i+2} & \dots & t_0 - t_{2i} \end{bmatrix},$$

where here and in the remaining part of this proof, we simply denote $t_j^{(q-1)}$ by t_j for any nonnegative integer index j.

Because of (2.16) the equalities $B_q(i, 1:i-1) = A_q(i, i:i-1)$, $i = 1, 2, \dots, \lfloor q/2 \rfloor$, are equivalent to the relations

$$t_{i-1}^{(q)} - t_{i+1}^{(q)} = t_{i-1} - t_{i+1} + t_{i-2} - t_{i+2} = (t_{i-2} + t_{i-1} + t_i) - (t_i + t_{i+1} + t_{i+2}),$$

and, for $k = 2, \dots, i-1$,

$$\begin{aligned} t_{i-k}^{(q)} - t_{i+k}^{(q)} &= (t_{i-k+1} - t_{i+k-1}) + (t_{i-k} - t_{i+k}) + (t_{i-k+1} - t_{i-k+2}) \\ &= (t_{i-k-1} + t_{i-k} + t_{i-k+1}) - (t_{i+k-1} + t_{i+k} + t_{i+k+1}), \end{aligned}$$

which follow from (2.20).

For the diagonal entries, for $i = 1, 2, \dots, \lfloor q/2 \rfloor$, we have

$$A_q(i,i) = t_0^{(q)} - t_{2i}^{(q)}, \qquad i = 1, 2, \dots, \lfloor q/2 \rfloor$$

and

$$\begin{aligned} A_{q-1}(1, 1:2) &= \begin{bmatrix} t_0 - t_2 & t_1 - t_3^{(q)} \end{bmatrix}, \\ A_{q-1}(i, i-1:i+1) &= \begin{bmatrix} t_1 - t_{2i-1} & t_0 - t_{2i} & t_1 - t_{2i+1}^{(q)} \end{bmatrix}, & i = 2, \dots, [q/2] - 1, \\ A_{q-1}(i, i-1:i+1) &= \begin{bmatrix} t_1 - t_{2i-1} & t_0 - t_{2i} & t_1 \end{bmatrix}, & 2i = q, \\ A_{q-1}(i, i-1:i+1) &= \begin{bmatrix} t_1 - t_{2i-1} & t_0 & t_1 \end{bmatrix}, & 2i+1 = q. \end{aligned}$$

Because of (2.16) and (2.10) the identities $B_q(i,i) = A_q(i, i:i)$, $i = 1, 2, \dots, \lfloor q/2 \rfloor$, are equivalent to the relations

$$\begin{aligned} t_0^{(q)} - t_2^{(q)} &= t_0 - t_2 + t_1 - t_3 + \delta_q = t_0^{(q)} - (t_1 + t_2 + t_3), \\ t_0^{(q)} - t_{2i}^{(q)} &= 2t_1 - t_0 - (t_{2i-1} + t_{2i} + (t_{2i+1}) + \delta_q \\ &= t_0^{(q)} - (t_{2i-1} + t_{2i} + t_{2i+1}), & i = 2, \dots, \lfloor q/2 \rfloor - 1, \\ t_0^{(q)} - t_{2i}^{(q)} &= 2t_1 - t_0 - (t_{2i-1} + t_{2i}) + \delta_q \\ &= t_0^{(q)} - (t_{2i-1} + t_{2i}), & 2i+1 = q, \\ t_0^{(q)} - t_{2i}^{(q)} &= 2t_1 - t_0 - (t_{2i-1} + t_{2i}) + \delta_q \\ &= t_0^{(q)} - t_{2i-1}, & 2i = q, \end{aligned}$$

ETNA
Kent State University and
Johann Radon Institute (RICAM)

which follow from (2.20) as above. In the same way we verify the cases $i = N - \lfloor q/2 \rfloor, \ldots, N$. Moreover, in a similar way, we may treat the remaining cases. □

The recursive description (2.9) of A_q and formula (2.8), will permit us to find in the next section a closed formula for the eigenvalues of the perturbation matrix A_q of a Toeplitz matrix T_q.

3. The spectrum of the perturbed matrices. Notice that if two $N \times N$ matrices B and C share the same eigenvectors, then the matrix BC also has the same eigenvectors and its eigenvalues are the products of the corresponding eigenvalues of B and C. The same properties are kept if we add to the matrix BC a scalar matrix, i.e., a scalar multiple of the identity matrix I_N. More precisely, if α is a number, then the common eigenvector x_k of B and C is an eigenvector of the matrix $BC + \alpha I$ with the corresponding eigenvalue $\lambda_k^C \lambda_k^B + \alpha$. Based on this, we obtain from the above results explicit formulas to determine the eigenvalues of the perturbed matrices A_k, $k = 1, 2, \ldots$

The next formula (3.1) is the same as formula (1.3), only that we now deal with more than a single perturbed matrix, and that is why we added an upper index that indicates the bandwidth of the perturbed matrix. The following is one of the main results of this paper.

THEOREM 3.1. *Let T_q be a q-band symmetric Toeplitz matrix with the only nonzero entries $T_q(i,j) = t_{|i-j|}^{(q)}$, $|i-j| \le q$, and with the last Toeplitz coefficient $t_q^{(q)} > 0$, and let A_q be the corresponding perturbed matrix from* (1.1).

The eigenvalues of A_q are

$$t_0^{(q)} + 2\sum_{j=1}^{q} t_j^{(q)} \cos\left(\frac{jk\pi}{N+1}\right), \qquad k = 1, \ldots, N. \tag{3.1}$$

Proof. Using formulas (2.8), determine, for $m = q-1, \ldots, 1$, the parameters $t_j^{(m)}$, $j = 0, 1, \ldots, m$, which define the band Toeplitz matrices T_m. Notice that the first formula in (2.20) implies

$$t_q^{(q)} = t_{q-1}^{(q-1)} = \cdots = t_1^{(1)} > 0.$$

By Theorem 2.1 the sequence of the corresponding perturbed matrices A_m, $m = 1, 2, \ldots, q$, satisfy the recursive relations (2.9), (2.10). We prove by induction on m that the eigenvalues of the matrices A_m, $m = 1, 2, \ldots,$ are

$$\lambda_k(A_m) = t_0^{(m)} + 2\sum_{j=1}^{m} t_j^{(m)} \cos(j\alpha_k), \qquad k = 1, \ldots, N, \tag{3.2}$$

with $\alpha_k = (k\pi)/(N+1)$.

For $m = 1$ we have $A_1 = T_1$, and (3.2) follows directly from (2.2) with $t_1 = t^{(1)} > 0$. Assume that for some $m \ge 1$ the relations (3.2) hold. Using (2.9) we have

$$\lambda_k(A_{m+1}) = \lambda_k(A_m)\lambda_k(T_M) + \delta_m, \qquad k = 1, 2, \ldots, N.$$

Hence, using (3.2), (2.3), and (2.10)

$$\lambda_k(A_{m+1}) = \left(t_0^{(m)} + 2\sum_{j=1}^{m} t_j^{(m)} \cos(j\alpha_k)\right)(1 + 2\cos(\alpha_k)) + t_0^{(m+1)} - 2t_1^{(m)} - t_0^{(m)},$$

i.e.,

$$\begin{aligned}\lambda_k(A_{m+1}) = 2\sum_{j=1}^{m} t_j^{(m)}\cos(j\alpha_k) + 2t_0^{(m)}\cos(\alpha_k)\\ + 4\sum_{j=1}^{m} t_j^{(m)}\cos(j\alpha_k)\cos(\alpha_k) - 2t_1^{(m)} + t_0^{(m+1)}.\end{aligned} \tag{3.3}$$

We have

$$\begin{aligned}4\sum_{j=1}^{m} t_j^{(m)}\cos(j\alpha_k)\cos(\alpha_k) &= 2\sum_{j=1}^{m} t_j^{(m)}\cos(j+1)\alpha_k + 2\sum_{j=1}^{m} t_j^{(m)}\cos(j-1)\alpha_k\\ &= 2\sum_{j=2}^{m+1} t_{j-1}^{(m)}\cos(j\alpha_k) + 2\sum_{j=0}^{m-1} t_{j+1}^{(m)}\cos(j\alpha_k)\\ &= 2\sum_{j=1}^{m+1} t_{j-1}^{(m)}\cos(j\alpha_k) + 2\sum_{j=1}^{m-1} t_{j+1}^{(m)}\cos(j\alpha_k) - 2t_0^{(m)}\cos(\alpha_k) + 2t_1^{(m)}.\end{aligned}$$

Inserting this into (3.3) we get

$$\begin{aligned}\lambda_k(A_{m+1}) = t_0^{(m+1)} + 2\sum_{j=1}^{m-1}(t_j^{(m)} + t_{j-1}^{(m)} + t_{j+1}^{(m)})\cos(j\alpha_k)\\ + 2(t_m^{(m)} + t_{m-1}^{(m)})\cos(m\alpha_k) + 2t_m^{(m)}\cos(m+1)\alpha_k.\end{aligned}$$

Hence, using (2.20), we obtain

$$\lambda_k(A_{m+1}) = t_0^{(m+1)} + 2\sum_{j=1}^{m+1} t_j^{(m+1)}\cos(j\alpha_k), \qquad k = 1,\dots,N,$$

which completes the proof □

The eigenvalues of the perturbed matrix A_q of a q-band symmetric Toeplitz matrix T_q, which have been obtained in this section in formula (3.1), will be used in the next section to establish bounds for each of the eigenvalues of T_q by proving an interlacing property between the eigenvalues of A_q and T_q.

4. Bounds and the interlacing property.

4.1. Overall bounds. To start the bisection algorithm we need to get initial lower and upper bounds B_L and B_U of the eigenvalues of the matrix. For the $N \times N$ q-band symmetric Toeplitz matrix T_q, one can take

$$B_L = -\|T_q\|_F, \qquad B_U = \|T_q\|_F,$$

where $\|T_q\|_F$ is the Frobenius (standard, trace) norm of T_q, which is readily computed as

$$\|T_q\|_F = \sqrt{Nt_0^2 + 2\sum_{k=1}^{q}(N-k)t_k^2}\,. \tag{4.1}$$

Of course, the norm

$$\|T_q\|_2 = \sqrt{\sup_{x\in\mathbb{R}^N} \frac{\sum_{k=1}^N |(T_q x)_k|^2}{\sum_{k=1}^N |x_k|^2}}$$

would suit best since for symmetric matrices it is equal to the largest absolute value of the eigenvalues of T_q so that no sharper bound can be found, but this norm is not easily computable for T_q.

Other bounds are obtained from the Gershgorin Theorem (see [20, Theorem 6.9.4] or [18, Ch. 6]), which in this case become

$$t_0 \pm 2\sum_{k=1}^{q} |t_k|. \tag{4.2}$$

The norms

$$\|T_q\|_1 = \max_{1\le j\le N} \sum_{i=1}^N |T_q(i,j)| = |t_0| + 2\sum_{k=1}^q |t_k|$$

and

$$\|T_q\|_\infty = \max_{1\le i\le N} \sum_{j=1}^N |T_q(i,j)| = |t_0| + 2\sum_{k=1}^q |t_k|$$

also are in fact equal to (4.2) if we take $t_0 = 0$, which we can suppose for now since otherwise we would find the same eigenvalues except for a t_0-shift.

Other lower and upper bounds for the eigenvalues of the matrix T_q, which is equal to $A_q + H_q$, are the sums of the smallest and, respectively, largest eigenvalues of these two matrices ([26, 17]) since the largest eigenvalue of the matrix sum is at most the sum of each of the two individual largest eigenvalues and it is equal to this sum only when their corresponding eigenvectors coincide. The same stands for the smallest eigenvalues. Therefore, we can take

$$\lambda_1^A + \lambda_1^H \le \lambda_k^T \le \lambda_N^A + \lambda_{q-1}^H, \qquad k = 1,\dots,N, \tag{4.3}$$

where for 2-band matrices we take $\lambda_1^H = 0$ and $\lambda_{q-1}^H = T_2(1,3)$. To this end, we can either compute the eigenvalues of the (small) matrix $\widetilde{H_q} = H_q(1:q-1, 1:q-1)$, or we can find a lower and an upper bound for its eigenvalues by applying, for instance, the Gershgorin Theorem to the small $(q-1)\times(q-1)$ matrix alone.

Since we plan to further find the eigenvalues of T_q by the method of bisection using Sturm polynomials and computing them all in a linear number of operations, it is much cheaper to start with the most suited overall interval. We obtained the left-hand value of this interval by computing all the above lower bounds (4.1)–(4.3) and then taking their maximum, while for the right-hand value of the bounding interval we took the minimum of the upper bounds that have been described above in (4.1)–(4.3).

4.2. The interlacing property with the perturbed matrices. The overall difference between the eigenvalues of a given q-band symmetric Toeplitz $N\times N$ matrix T_q and its perturbed matrix A_q is

$$\sum_{k=1}^N (\lambda_k^{T_q} - \lambda_k^{A_q}) = 2\sum_{m=1}^{\lfloor q/2\rfloor} t_{2m}^{(q)},$$

where $t_j^{(q)} = T_q(j+1, 1)$, since the last sum is the trace of the matrix H_q.

The following theorem is from [15, p. 443] and its proof can be found in [28, pp. 104–108].

THEOREM 4.1 (Wielandt-Hoffman [16]). *If A and $A+H$ are $N\times N$ symmetric matrices, then the square of the distances between their eigenvalues satisfy*

$$\sum_{k=1}^{N}(\lambda_k^{A+H}-\lambda_k^{A})^2 \leq \|H\|_F^2.$$

Here $\|H\|_F$ denotes the Frobenius norm of the matrix H.

Since the q-band symmetric Toeplitz matrix T_q, $q\geq 2$, differs from the perturbed matrix A_q only by the entries

$$A_q(i,j)=T_q(i,j)-t_{i+j}, \qquad \text{where} \quad i+j\leq q, \quad \text{or} \quad i+j\geq 2N-q+2,$$

it follows that the square of the Frobenius norm of the perturbation matrix H_q, which is also equal to the sum of the squares of all the entries of H_q, is $2\sum_{j=1}^{q-1} jt_{j+1}^2$ so that

$$\sum_{k=1}^{N}(\lambda_k^{T}-\lambda_k^{A})^2 \leq 2\sum_{j=1}^{q-1} jt_{j+1}^2, \tag{4.4}$$

as we mentioned in the introduction, and the right-hand side is independent of the size N.

Next in this section, we obtain the interlacing inequalities (1.4) between the eigenvalues of the matrix T_q and the perturbed matrix A_q. The general theorem we used is based upon [15, Theorem 8.1.8, p. 443], and its proof can be found in [28, pp. 94–97].

THEOREM 4.2. *If A is an $N\times N$ symmetric matrix with its eigenvalues sorted in ascending order, c is an N-dimensional column vector with real entries and unit Euclidean norm, and $B=A+\beta cc^T$, where $\beta\in\mathbb{R}$, then, if $\beta\geq 0$,*

$$\lambda_k^{A}\leq\lambda_k^{B}\leq\lambda_{k+1}^{A}, \qquad k=1,\ldots,N-1, \tag{4.5}$$

while if $\beta\leq 0$,

$$\lambda_{k-1}^{A}\leq\lambda_k^{B}\leq\lambda_{k}^{A}, \qquad k=2,\ldots,N. \tag{4.6}$$

Based on this theorem we obtain the following interlacing properties for the symmetric matrices T_q and A_q. An $r\times r$ matrix S is called *strongly regular* if all its principal leading submatrices are regular, i.e., $\det S(1:m,1:m)\neq 0$, $m=1,\ldots,r$.

THEOREM 4.3. *Let T be a q-band symmetric Toeplitz matrix with the corresponding perturbed matrix A. Assume that the matrix*

$$H=T(1:q-1,1:q-1)-A(1:q-1,1:q-1)$$

is strongly regular, and denote by n the number of its negative eigenvalues and by $p=q-1-n$ the number of its positive eigenvalues (including multiplicities).

Then

$$\lambda_{k-2n}^{A}\leq\lambda_k^{T}\leq\lambda_{k+2p}^{A}, \qquad k=2n+1,\ldots,N-2p. \tag{4.7}$$

(Here we repeated formula (1.4) from the introduction.) In the proof we use a representation of a strongly regular matrix as a sum of rank-one matrices.

LEMMA 4.4. *Let S be an $m \times m$ strongly regular matrix, let $\gamma_0 = 1$, and let $\gamma_1, \dots, \gamma_m$ be the determinants of its principal leading submatrices, i.e., $\gamma_j = \det S(1:j, 1:j) \neq 0$, $j = 1, \dots, m$. Then,*

$$S = \sum_{k=1}^{m} \frac{\gamma_k}{\gamma_{k-1}} c_k b_k^T \tag{4.8}$$

with m-dimensional column vectors c_k, b_k that will be specified in (4.9) below.

Proof. A strongly regular matrix S admits an LDU factorization (see, for instance, [7, Section 1.6]), where L is a lower triangular matrix which has ones on the main diagonal, D is a diagonal matrix with the nonzero entries $D_{kk} = \frac{\gamma_k}{\gamma_{k-1}}$, $k = 1, \dots, m$, and U is an upper triangular matrix having ones on its main diagonal. Thus, we obtain (4.8) with

$$c_k = \begin{bmatrix} 0_{k-1} \\ 1 \\ L(k+1:m, k) \end{bmatrix}, \qquad b_k^T = \begin{bmatrix} 0_{k-1} & 1 & U(k, k+1:m) \end{bmatrix}, \tag{4.9}$$

which completes the proof □

Proof of Theorem 4.3. As a difference of two symmetric matrices, H is symmetric, too. Hence, the representation (4.8) of the strongly regular matrix H has the form

$$H = \sum_{i=1}^{q-1} \frac{\gamma_i}{\gamma_{i-1}} c_i c_i^T. \tag{4.10}$$

Moreover, the number of negative values in the sequence of the quotients

$$\frac{\gamma_1}{\gamma_0}, \frac{\gamma_2}{\gamma_1}, \dots, \frac{\gamma_{q-1}}{\gamma_{q-2}}$$

equals the number of the negative eigenvalues of the matrix H. So the numbers of positive and negative coefficients in the sum (4.10) are equal to the numbers n and $p = q - n - 1$ of negative and positive eigenvalues of H. Of course, one has to normalize the vectors in (4.8) in order to apply Theorem 4.2, but scaling and then multiplying with norms does not change the sign of the coefficient in front of the vectors in the sum.

The matrix T_q is a perturbation of the matrix A_q by two strongly regular diagonal blocks of size $(q-1) \times (q-1)$ with n negative eigenvalues and $p = q - n - 1$ positive eigenvalues. This means that

$$T_q = A_q + \sum_{j=1}^{2p} \beta_j c_j c_j^T - \sum_{j=1}^{2n} \alpha_j b_j b_j^T.$$

Set $A = A_q$ and

$$B = A + \beta_1 c_1 c_1^T, \qquad D = B + \beta_2 c_2 c_2^T.$$

Using (4.5) we get

$$\lambda_k^A \leq \lambda_k^B, \quad \lambda_{k+1}^B \leq \lambda_{k+2}^A, \qquad k = 1, \dots, N-2$$

and

$$\lambda_k^B \leq \lambda_k^D \leq \lambda_{k+1}^B, \qquad k = 1, \dots, N-1.$$

ETNA
Kent State University and
Johann Radon Institute (RICAM)

Hence,

$$\lambda_k^A \le \lambda_k^B \le \lambda_k^D \le \lambda_{k+1}^B \le \lambda_{k+2}^A, \qquad k = 1, \dots, N-2,$$

which after discarding the intermediate entries assures that

$$\lambda_k^A \le \lambda_k^D \le \lambda_{k+2}^A, \qquad k = 1, \dots, N-2.$$

Using the formula (4.5) $2p-1$ times in a row, we obtain

$$\lambda_k^A \le \lambda_k^F \le \lambda_{k+2p}^A, \qquad k = 1, \dots, N-2p, \tag{4.11}$$

where

$$F = A_q + \sum_{j=1}^{2p} \beta_j c_j c_j^T.$$

Next setting $C = F - \alpha_1 b_1 b_1^T$ and using (4.6) and (4.11), we obtain

$$\lambda_{k-2}^A \le \lambda_{k-2}^F \le \lambda_{k-1}^C \le \lambda_{k-1}^F \le \lambda_k^C \le \lambda_k^F \le \lambda_{k+2p}^A,$$

which implies

$$\lambda_{k-2}^A \le \lambda_{k-1}^C \le \lambda_{k+2p}^A.$$

Repeating these arguments $2n-1$ times in a row, we obtain (4.7). ∎

Numerical experiments show that at least for $2, 3, 4, 5$-band matrices, one cannot ask for a better interlacing property for the general case than the one obtained in Theorem 4.3. For instance, if $N = 1024$, $q = 2$, and $t_0 = 0$, $t_1 = 1$, $t_2 = 2$, some of the nondecreasing eigenvalues λ_k^T of T_2 are between λ_k^A and λ_{k+1}^A and some are between λ_{k+1}^A and λ_{k+2}^A.

REMARK 4.5. Note that by the same proof one can show that if any two Hermitian matrices B and C differ only in a (Hermitian) diagonal $m \times m$ strongly regular block that has p_1 positive eigenvalues and $n_1 = m - p_1$ negative eigenvalues, then their eigenvalues satisfy the interlacing property

$$\lambda_{k-n_1}^B \le \lambda_k^C \le \lambda_{k+p_1}^B, \qquad k = n_1 + 1, \dots, N - p_1.$$

Denote by J_m the $m \times m$ matrix which has the only nonzero entries equal to 1 located on the counter-diagonal. Then note also that, by a slight modification of the proof, one can show that if the lower parts of any two Hermitian matrices B and C differ only in an (off-diagonal) $m \times m$ block M such that the block M or MJ_m or $J_m M$ is Hermitian and strongly regular and it has p_1 positive eigenvalues and $n_1 = m - p_1$ negative eigenvalues, then the eigenvalues of B and C satisfy the interlacing property

$$\lambda_{k-(p_1+2n_1)}^B \le \lambda_k^C \le \lambda_{k+2p_1+n_1}^B, \qquad k = p_1 + 2n_1 + 1, \dots, N - 2p_1 - n_1.$$

In the next section we will use the interlacing property that has been proved in this section and the exact eigenvalues of A_q that have been obtained in Section 3 to find the eigenvalues of T_q by the method of bisection in a faster way.

5. Finding the eigenvalues by the method of bisection. In this section, for band symmetric Toeplitz matrices, we specify a general method to compute eigenvalues and eigenvectors that was developed in [11] for Hermitian matrices with quasiseparable representations.

ETNA
Kent State University and
Johann Radon Institute (RICAM)

5.1. The quasiseparable representation. The following definitions and further information can be found, for instance, in Part I of the book [7]. Let $\{a(k)\}$ be a family of matrices of sizes $r_k \times r_{k-1}$. For positive integers i, j, $i > j$, define the operation $a^{>}_{ij}$ as follows:

$$a^{>}_{ij} = \begin{cases} a(i-1) \cdot \ldots \cdot a(j+1) & \text{for } i > j+1, \\ a^{>}_{j+1,j} = I_{r_j}. \end{cases}$$

Let $\{b(k)\}$ be a family of matrices of sizes $r_{k-1} \times r_k$. For positive integers i, j, $j > i$, define the operation $b^{<}_{ij}$ as follows:

$$b^{<}_{ij} = \begin{cases} b(i+1) \cdot \ldots \cdot b(j-1) & \text{for } j > i+1, \\ b^{<}_{i,i+1} = I_{r_i}. \end{cases}$$

Let $A = \{A_{ij}\}_{i,j=1}^{N}$ be a matrix with scalar entries A_{ij}. Assume that the entries of this matrix are represented in the form

$$A_{ij} = \begin{cases} p(i)a^{>}_{ij}q(j), & 1 \le j < i \le N, \\ d(i), & 1 \le i = j \le N, \\ g(i)b^{<}_{ij}h(j), & 1 \le i < j \le N. \end{cases} \tag{5.1}$$

Here

$$p(i)\ (i = 2, \ldots, N), \qquad q(j)\ (j = 1, \ldots, N-1), \qquad a(k)\ (k = 2, \ldots, N-1)$$

are matrices of sizes $1 \times r^L_{i-1}$, $r^L_j \times 1$, $r^L_k \times r^L_{k-1}$, respectively,

$$g(i)\ (i = 1, \ldots, N-1), \qquad h(j)\ (j = 2, \ldots, N), \qquad b(k)\ (k = 2, \ldots, N-1)$$

are matrices of sizes $1 \times r^U_i$, $r^U_{j-1} \times 1$, $r^U_{k-1} \times r^U_k$, respectively, and $d(i)\ (i = 1, \ldots, N)$ are (possibly complex) numbers.

The representation of a matrix A in the form (5.1) is called a *quasiseparable representation*. The elements

$$\begin{array}{lll} p(i)\ (i = 2, \ldots, N), & q(j)\ (j = 1, \ldots, N-1), & a(k)\ (k = 2, \ldots, N-1), \\ g(i)\ (i = 1, \ldots, N-1), & h(j)\ (j = 2, \ldots, N), & b(k)\ (k = 2, \ldots, N-1,) \\ d(i)\ (i = 1, \ldots, N) & & \end{array}$$

are called *quasiseparable generators* of the matrix A. The numbers $r^L_k, r^U_k\ (k = 1, \ldots, N-1)$ are called the *orders* of these generators. The elements

$$\begin{array}{lll} p(i)\ (i = 2, \ldots, N), & q(j)\ (j = 1, \ldots, N-1), & a(k)\ (k = 2, \ldots, N-1), \\ g(i)\ (i = 1, \ldots, N-1), & h(j)\ (j = 2, \ldots, N), & b(k)\ (k = 2, \ldots, N-1) \end{array}$$

are also called *lower quasiseparable generators* and *upper quasiseparable generators* of the matrix A. In fact the generators $p(i), g(i)$ and $q(j), h(j)$ are row and column vectors of corresponding sizes.

For a Hermitian matrix the diagonal entries $d(k)\ (k = 1, \ldots, N)$ are real, and moreover, the upper quasiseparable generators can be obtained from the lower ones by taking

$$\begin{array}{llll} g(k) = (q(k))^*, & h(k) = (p(k))^*, & b(k) = (a(k))^*, & k = 2, \ldots, N-1, \\ g(1) = (q(1))^*, & h(N) = (p(N))^*. & & \end{array}$$

ETNA
Kent State University and
Johann Radon Institute (RICAM)

A matrix $A = \{A_{ij}\}_{i,j=1}^N$ is said to be an r-band matrix if $A_{ij} = 0$, $|i-j| > r$. Such a matrix has quasiseparable representations with orders equal r. Quasiseparable representations for any band matrices can be found, e.g., in [7, p. 81]. For instance, for a 3-band quasiseparable matrix, the lower quasiseparable generators are

$$p(i) = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix},\ i = 2,\dots,N, \qquad q(j) = \begin{bmatrix} A_{j+1,j} \\ A_{j+2,j} \\ A_{j+3,j} \end{bmatrix},\ j = 1,\dots,N-1; \tag{5.2}$$

$$a(k) = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix},\ k = 2,\dots,N-1. \tag{5.3}$$

The matrix entries $A_{N+1,N-2}$, $A_{N+1,N-1}$, and $A_{N+2,N-1}$ are here supposed to be zero.

An m-band symmetric Toeplitz matrix has the lower quasiseparable generators

$$\begin{aligned} p(i) &= \begin{bmatrix} 1 & 0 & \dots & 0 \end{bmatrix}, & i &= 2,\dots,N, \\ q(j) &= \begin{bmatrix} t_1 & t_2 & \dots & t_m \end{bmatrix}^T, & j &= 1,\dots,N-1; \end{aligned} \tag{5.4}$$

$$a(k) = \begin{bmatrix} 0 & 1 & \dots & 0 \\ \vdots & & \ddots & \\ \vdots & & & 1 \\ 0 & \dots & \dots & 0 \end{bmatrix}, \qquad k = 2,\dots,N-1, \tag{5.5}$$

and the diagonal entries

$$d(k) = t_0, \qquad k = 1,\dots,N. \tag{5.6}$$

5.2. Find the number ν of sign changes in the Sturm sequence. The basic part of the bisection algorithm is the computation of the number of negative entries in the Sturm sequence

$$D_k(\lambda) = \frac{\gamma_k(\lambda)}{\gamma_{k-1}(\lambda)}, \qquad k = 1,2,\dots,N, \tag{5.7}$$

where $\gamma_0(\lambda) \equiv 1$, $\gamma_1(\lambda), \gamma_2(\lambda), \dots, \gamma_N(\lambda)$ are characteristic polynomials of the principal leading submatrices of a matrix. In our case this number is obtained as follows.

The algorithm presented in [7, Theorem 18.2] yields in particular the ratios of the determinants of the principal leading submatrices of a matrix A with a given quasiseparable representation. Applying this result to the matrix $A - \lambda I$, we obtain recursive relations for the functions in the sequence (5.7). For the Hermitian matrix A with lower quasiseparable generators

$$p(i)\ (i = 2,\dots,N), \qquad q(j)\ (j = 1,\dots,N-1), \qquad a(k)\ (k = 2,\dots,N-1)$$

ETNA
Kent State University and
Johann Radon Institute (RICAM)

of orders r_k^L $(k = 1, \dots, N-1)$ and diagonal entries $d(k)$ $(k = 1, \dots, N)$ and for the real number λ, one obtains the recursive relations

$$D_1(\lambda) = d(1) - \lambda, \qquad u_1(\lambda) = q_1 \frac{1}{D_1(\lambda)}, \qquad f_1 = u_1(\lambda) q^*(1);$$

$$\left.\begin{aligned} D_k(\lambda) &= d(k) - \lambda - p(k) f_{k-1}(\lambda) p^*(k), \\ u_k(\lambda) &= [q(k) - a(k) f_{k-1}(\lambda) p^*(k)] \frac{1}{D_k(\lambda)}, \\ f_k(\lambda) &= a(k) f_{k-1}(\lambda) a^*(k) + u_k(\lambda) q^*(k) - p(k) f_{k-1}(\lambda) a^*(k)], \end{aligned}\right\} \quad k = 2, \dots, N-1;$$

$$D_N(\lambda) = d(N) - \lambda - p(N) f_{N-1}(\lambda) p^*(N).$$

Inserting (5.4), (5.5), (5.6) in these relations and counting the negative entries in the sequence (5.7), we obtain the following procedure.

ALGORITHM 5.1 (**Find ν**).
The number ν of sign changes in the Sturm sequence for a given real value λ and for an $N \times N$ m-band symmetric Toeplitz matrix T_m, with a given diagonal entry $d \equiv t_0$ and a given row vector $q = (t_1, \dots, t_m)$ of Toeplitz coefficients, is computed by the following steps.

1. Compute $\delta = d - \lambda$, $u_1 = q^T/\delta$, $f_1 = u_1 q$.
   Set $\nu = 1$ if $\delta < 0$ and $\nu = 0$ otherwise.
2. For $k = 2, \dots, N-1$ compute

$$D_k = \delta - f_{k-1}(1,1),$$
$$\phi_k = \begin{bmatrix} q(1:m-1) - f_{k-1}(2:m,1) \\ q(m) \end{bmatrix}, \qquad u_k = \phi_k / D_k,$$
$$f_k = \begin{bmatrix} f_{k-1}(2:m, 2:m) & 0_{(m-1)\times 1} \\ 0_{1\times(m-1)} & 0 \end{bmatrix} + u_k \phi_k^T.$$

   Set $\nu = \nu + 1$ if $D_k < 0$.
3. Set $\nu = \nu + 1$ if $\delta - f_{N-1}(1,1) < 0$.

Here we used the fact that the generators in (5.3) and their transposes represent a right shift and an upwards shift, respectively, and the generators in (5.2) perform simple actions as well. An optimized version with the same input follows in Algorithm 5.2. It requires less memory and also less operations.

ALGORITHM 5.2.

1. Compute $r = m - 1$, $\delta = d - \lambda$, $v = q^T/\delta$, $f = vq$.
   Set $v(m) = q(m)$, and set $\nu = 1$ if $\delta < 0$ and $\nu = 0$ otherwise.
2. Compute $N - 2$ times

$$D = \delta - f(1,1), \qquad v(1:r) = q(1:r)^T - f(2:m,1), \qquad \text{and}$$
$$\varphi = vv^T/D, \quad \varphi(1:r,1:r) = \varphi(1:r,1:r) + f(2:m,2:m), \quad f = \varphi.$$

   Set each time $\nu = \nu + 1$ if $D < 0$.
3. Set $\nu = \nu + 1$ if $\delta - f(1,1) < 0$.

The complexity of the above algorithm is $2 + m + m^2$ entrywise arithmetical operations (besides assignments) for the first step, $(1 + (m-1) + 2m^2 + (m-1)^2 + 1.5)(N-2)$ for the main step (besides the loop counter), and 1.5 for the third step, so that the overall complexity is less than

$$c_\nu = (3m^2 - m + 2.5)N$$

ETNA
Kent State University and
Johann Radon Institute (RICAM)

for an $N \times N$ symmetric m-band matrix. Its complexity is of high importance since this algorithm is extensively used in our computations.

5.3. Algorithm for separating eigenvalues. The initial bounds for the eigenvalues of T_m are given by an overall lower bound at the left (like minus the Frobenius norm), an overall upper bound, and, in between them, the N eigenvalues of the perturbed matrix A_m sorted in ascending order. Between any two consecutive such lower and upper bounds there can be more than one eigenvalue of T_m. In this case we use the algorithm in this section (see also step 4.2. of the complete algorithm in the next section) in order to refine the bounds for each eigenvalue of T_m separately.

ALGORITHM 5.3 (**Find lower and upper bounds for each eigenvalue**).
Lower and upper bounds $L_0(k), U_0(k)$ for each eigenvalue of an $N \times N$ m-band symmetric Toeplitz matrix T_m, with a given diagonal entry $d \equiv t_0$ and a given row vector $q = (t_1, \ldots, t_m)$ of off-diagonal Toeplitz coefficients, are received and renewed by the following steps. This algorithm also receives as input the number $n > 1$ of eigenvalues in the larger bounding interval and the number f of already found bounding intervals for smaller eigenvalues of T_m.

1. Compute $\lambda = (L_0(f+1) + U_0(f+n))/2$ and find ν for this λ by calling Algorithm 5.2.
   Compute $n_1 = \nu - f$ and $n_2 = n - n_1$.
2. For $j = 1, \ldots, n_1$ set $U_0(f+j) = \lambda$.
   Afterwards, if $n_1 > 1$ and $U_0(f+n_1) - L_0(f+1) > \varepsilon$, where ε denotes the machine precision, call again recursively this Algorithm 5.3 with n_1 instead of n.
3. For $j = n_1 + 1, \ldots, n$ set $L_0(f+j) = \lambda$.
   Afterwards, if $n_2 > 1$ and $U_0(f+n) - L_0(n_1+1) > \varepsilon$, call again recursively this Algorithm 5.3 with n_2 instead of n and ν instead of f.
4. Output the new lower and upper bounds.

5.4. The complete algorithm for finding all or selected eigenvalues. The next algorithm finds first specific lower and upper bounds $L_0(k), U_0(k)$, $k = 1, \ldots, N$, for each of the eigenvalues of the considered $N \times N$ Toeplitz matrix, based on interlacing properties between them and the eigenvalues of the perturbed matrix A. Then, it accelerates finding the precise value of each eigenvalue by bisecting between L_0 and U_0.

ALGORITHM 5.4 (**Find the eigenvalues $\boldsymbol{\lambda^T_{m_1}, \ldots, \lambda^T_{m_2}}$**).
This algorithm receives as input the real Toeplitz coefficients, namely the diagonal entry $d = t_0$ and the row vector $(t_1, \ldots, t_q)$ of size q of an $N \times N$ q-band symmetric Toeplitz matrix T_q. It finds the eigenvalues starting with the m_1 highest eigenvalue up to the m_2 highest eigenvalue. To this end, perform the following steps.

1. 1.1. Find a lower and an upper overall bound, say B_L and B_U, respectively, for all the eigenvalues of the q-band symmetric matrix T_q, like in Section 4.1. For instance, compute its Frobenius norm F from its $q+1$ Toeplitz coefficients by using formula (4.1) or the maximal absolute value of the two bounds from (4.2).
   1.2. Scale the matrix by dividing its $q+1$ Toeplitz coefficients by F. This will make all the eigenvalues sub-unitary and will prevent overflow. Denote them again by $t_0, t_1, \ldots, t_q$.
   1.3. If $t_q > 0$, then set $\sigma = 1$, else change the signs of all the $q+1$ Toeplitz coefficients, denote them again by $t_0, t_1, \ldots, t_q$, and set $\sigma = -1$.

   Thus, we have reduced the problem to another one with data suitable for the next computations.
2. Using the formulas (3.1), find the eigenvalues $\lambda_1^A, \ldots, \lambda_N^A$ of the perturbed matrix A_q and sort these numbers in ascending order. Denote them again by $\lambda_1^A, \ldots, \lambda_N^A$. Also take $\lambda_0^A = -1$, $\lambda_{N+1}^A = 1$.

3. Find the numbers n and p of negative and positive eigenvalues, respectively, of the strongly regular $(q-1)\times(q-1)$ Hankel matrix

$$H_q = T_q(1:q-1, 1:q-1) - A_q(1:q-1, 1:q-1).$$

   Note that
   - if $q=2$ we may set $n=0, p=1$,
   - if $q=3$ set $n=p=1$,
   - if $q=4$ set $n=1, p=2$,

   without any further computations.
   If $q=5$ and all the 3 expressions

$$t_2, \qquad t_2t_4 - t_3^2, \qquad 2t_3t_4t_5 - t_4^3 - t_2t_5^2$$

   are positive, then set $p=4$,
   else,
   if only $t_2t_4 - t_3^2$ is positive, then set $p=0$, else set $p=2$ and in all the cases set $n = q-1-p$.
4. Set $M_1 = \max\{m_1 - 2n, 0\}, M_2 = \min\{m_2 + 2p, N+1\}, s = M_2 - M_1 + 1$. With this s, for $k = 1, \ldots, s$, set $\lambda_k^0 = \lambda_{M_1+k-1}^A$.
   4.1. Set ν equal to the number of eigenvalues of T_q which are less than λ_1^0.
   4.2. For $k = 2, \ldots, s$ perform steps 4.2.1. to 4.2.3.
      4.2.1. Set ν_0 equal to the number of eigenvalues of T_q which are less than λ_k^0 and $n = \nu_0 - \nu$.
      If $n = 1$, then set the left (lower) and right (upper) bounds $L_0(\nu+1) = \lambda_{k-1}^0, U_0(\nu+1) = \lambda_k^0$.
      4.2.2. If $n > 1$, for $j = \nu+1, \ldots, \nu_0$, set $L_0(j) = \lambda_{k-1}^0, U_0(j) = \lambda_k^0$ and then, if $\nu < m_2$ and $\nu + n \geq m_1$, perform step 4.2.3.
      4.2.3. Find bounds $L_0(\nu+1:\nu+n)$, $U_0(\nu+1:\nu+n)$ with Algorithm 5.3.

   Thus, we have obtained lower and upper bounds for each of the (selected) eigenvalues.
5. 5.1. Denote by ε the machine precision.
   5.2. For $k = 1, \ldots, s$ compute the exact value of the eigenvalue

$$\lambda^T(k) \in [L_0(k), U_0(k)]$$

   by using genuine bisection as it was done in [15, p. 467] for symmetric tridiagonal matrices. Namely, perform the following steps.
      5.2.1. *While* $U_0(k) - L_0(k) < \varepsilon$:
      Set $\lambda = (U_0(k) + L_0(k))/2$.
      Compute with Algorithm 5.2 the number of sign changes ν in the Sturm sequence of T_q for the real number λ, and if $\nu = k$ set $U_0(k) = \lambda$ else set $L_0(k) = \lambda$.
      5.2.2. On exiting the *while* loop set

$$\lambda^T(k) = (U_0(k) + L_0(k))/2.$$

6. De-scale the eigenvalues by multiplying them with σF which has been computed in step 1.

5.5. Find the normalized eigenvector for a simple eigenvalue λ. Here we present an eigenvector algorithm. We are aware of the fact that usually this algorithm would not be stable because of the lack of orthogonality of the computed eigenvectors, but for the special case of band symmetric Toeplitz matrices it works very well.

ETNA
Kent State University and
Johann Radon Institute (RICAM)

ALGORITHM 5.5.
The normalized eigenvector for a given simple eigenvalue λ of an $N \times N$ m-band symmetric Toeplitz matrix T_m, with a given diagonal entry $d \equiv t_0$ and a given row vector $q = (t_1, \dots, t_m)^T$ of Toeplitz coefficients, is computed by the following steps.

0. Set $r = m-1$, $h_m = (N-\rho)/2$, where ρ is the remainder of the integer division of N by 2 and $h_p = h_m + 1$.
1. Using the recursive relations from Algorithm 5.1, find the column vectors u_k, for $k = 1, \dots, N-1$.
2. 2.1. Set $x(N) = 1$, $s_{N-1} = \begin{bmatrix} 1 \\ 0_{(m-1)\times 1} \end{bmatrix}$.
   2.2. For $k = N-1, N-2, \dots, h_m$, set $n = 1$ and perform:
$$x(k) = -u_k^T s_k, \quad s_{k-1} = \begin{bmatrix} x(k) \\ s_k(1:m-1) \end{bmatrix}, \quad n = n + (x(k))^2.$$
   2.3. Compute $n := \sqrt{2(n - (x(h_m))^2) - \rho(x(h_p))^2}$.
3. 3.1. Set $\sigma = 1$ if $x(h_m)x(h_p+\rho) > 0$ else $\sigma = -1$.
   3.2. For $j = h_p + 1, \dots, N$, set $x(N+1-j) = \sigma x(j)$.
   3.3. Normalize $x(1:N) = x(1:N)/n$.

REMARK 5.6. The steps up to 2.2. are a particular case of an algorithm from [11], only that step 2.2. is executed there up to $k = 2$ and not only up to h_m. But since the eigenvectors of our matrices are either symmetric or skew-symmetric (see [5]), we build the first half of the eigenvector from its already computed second half. The norm n of the eigenvector is also computed from only half of the vector in step 2.3.

6. Numerical experiments. All the numerical experiments, except for the first one, have been performed on a computer with an i7-5820 microprocessor, 31.9 gigabytes installed memory (RAM) at 3.30GHz and another 4GB at the video card GTX, which is exploited by Matlab as well. The operating system is Windows 10, 64 bits, the precision of the machine is 2.2204e-16, as given by the Matlab command eps, and the least positive number which is used by the machine is 2.2251E-308 as given by the Matlab command realmin.

We performed numerical tests for m-band matrices, where $m = 2$ to 7. For each tested band width, we built matrices with sizes $N \times N$, where N is a power of 2, either from $2^3 = 8$ up to $2^{11} = 2048$, or from 2^4 up to 2^{15}.

6.1. The computation time. The computation time for finding eigenvalues of the Toeplitz matrix (see Figure 6.1, left) was very low for 2-band matrices, for which special algorithms from the appendix were used. Among them was the function for finding the number ν of sign changes in the Sturm polynomials, which has been written with no use of vectorization, in which case Matlab is slower. For $m = 3, 4, 5$, we used the general algorithm, and finding the eigenvalues for $m = 3$ took 1000 times more time than for $m = 2$. As a comparison, it took only 20% more time for the order $m = 5$ than for $m = 3$.

The time to find all the eigenvectors was much lower than the time for finding all the eigenvalues. For 2-band matrices, due to the special algorithm, this time was practically zero (less than 0.001 seconds) even for a size of 2048, so that we do not plot it. We display the time for finding all the eigenvectors for $m = 3, 4, 5$ in Figure 6.1.

6.2. The error. The error for finding the eigenvalues (see Figure 6.2) has been computed by $\frac{1}{N}\sum_{k=1}^{N} |\lambda(k) - \lambda_M(k)|$, i.e., the average of the absolute value of the difference between our eigenvalues and the eigenvalues computed by Matlab, $\lambda_M(k)$, $k = 1, \dots, N$, of the same matrix. The error for finding the eigenvectors has been computed as the average entry of the

ETNA
Kent State University and
Johann Radon Institute (RICAM)

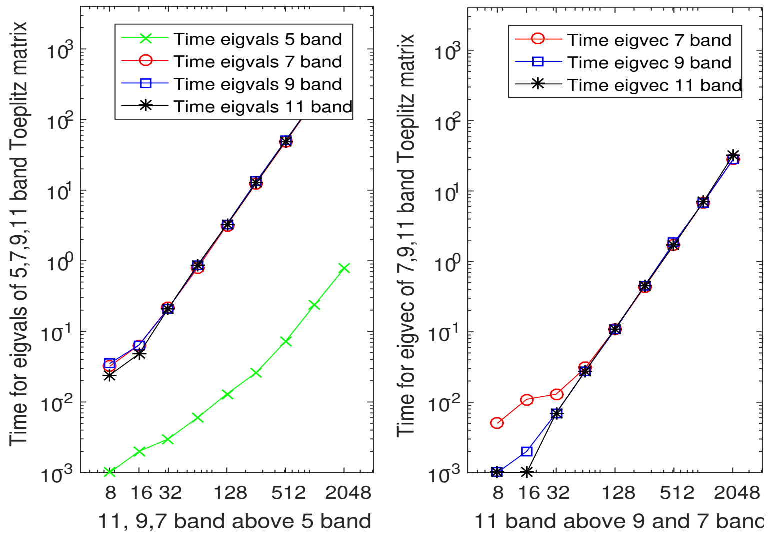

FIG. 6.1. *The time for finding the eigenvalues (left figure) and eigenvectors (at the right) has been tested on purpose on a very slow computer.*

vectors $Tx - \lambda x$, namely as $\frac{1}{N^2}\sum_{j,k=1}^{N} |Tx_k(j) - \lambda_k x_k(j)|$, where T is the Toeplitz matrix, λ_k is an eigenvalue, and x_k is its corresponding eigenvector.

6.3. Cluster of eigenvalues. The time for finding, with linear complexity, the eigenvalues of the perturbed matrix A was less than 0.001 seconds even when we tested this on a much slower computer and even for matrices $N = 2048$ and $m = 5$. On the faster computer described above, computing recursively and sorting all the eigenvalues of the perturbed matrix took 0.001 seconds for matrices of size 32768×32768 and for 3-band matrices. Of course, we used the $\cos$ function only $\left\lfloor \frac{N}{2} \right\rfloor$ times, and we used them with $\pm$ to build all the necessary cosines. The error for our eigenvalues for A when compared with Matlab's eigenvalues has never been larger than two times the machine precision on our machine. So we did not plot neither the time nor the error, as we did not plot zero numbers.

Thus, for a cluster of s consecutive eigenvalues of an m-band symmetric Toeplitz matrix T, we obtain in no time $s+2m-2$ consecutive eigenvalues of the perturbed matrix A, between which the wanted eigenvalues of T hide. Then, we find them in linear time. When we verified the algorithm for finding a cluster of 5 selected eigenvalues, we obtained for any one of them an error which is less than machine precision, even for $N = 2048$.

6.4. Orthogonality of all the eigenvectors. In order to find the orthogonality error for the eigenvectors (see Figure 6.3), we tested the average absolute entry of the matrix $I_N - X^T X$, where X is the matrix that has our normalized eigenvectors as its columns. Namely, we plot for a matrix of size $N \times N$ the number

$$\frac{1}{N^2}\left(2\sum_{1\le j<i\le N} |(X^T X)_{i,j}| + \sum_{i=1}^{N} |(X^T X)_{i,i} - 1|\right).$$

The sizes of the matrices are powers of 2, from 2^4 up to 2^{15} for 2-band matrices and up to 2^{13} for 5-band and 7-band matrices. The orthogonality of the eigenvectors built through our method is known to be poor for large matrices [11], but here, for band symmetric Toeplitz matrices, which have real quasiseparable generators, the entries of which are mostly all 0 or 1

ETNA
Kent State University and
Johann Radon Institute (RICAM)

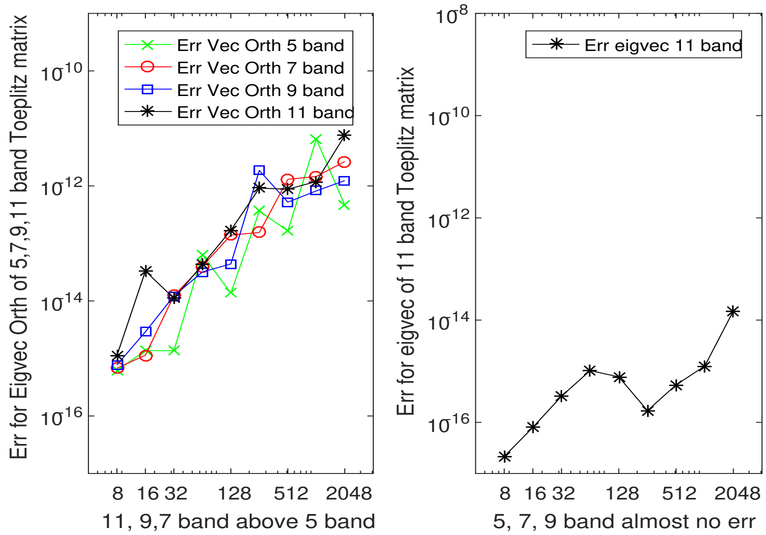

FIG. 6.2. *Errors in finding the eigenvalues (left) and eigenvectors (right).*

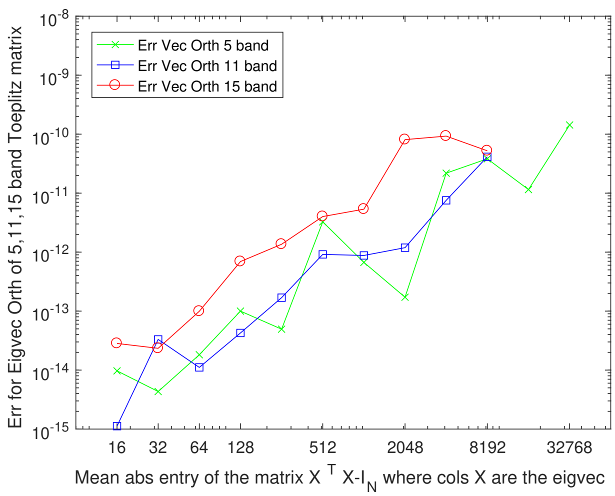

FIG. 6.3. *In this figure, we verified the orthogonality of the eigenvectors by plotting the average absolute entry of the matrix $X^T X - I_N$, where the columns of X are the normalized eigenvectors.*

and thus contribute no error in the multiplications, the eigenvectors prove to be almost exact for huge matrices also.

6.5. All the eigenstructure. Finally, we tested all our eigendata at once (see Figure 6.4) by plotting the spectral norm of the matrix $X^T T X - \mathrm{diag}(\lambda_1, \ldots, \lambda_N)$, where the columns of the matrix X are the eigenvectors corresponding to the respective eigenvalues that we found and which form the diagonal matrix mentioned in the formula. The eigendata are exact, even with our demanding way to find the error. Since computing the plotted parameter takes a lot of time, we did it up to matrices of size $2^{15} = 32768$ only for 2-band matrices and for 5-band and 7-band only for matrices up to size 1024.

The code of the program is available from the authors on email request.

ETNA
Kent State University and
Johann Radon Institute (RICAM)

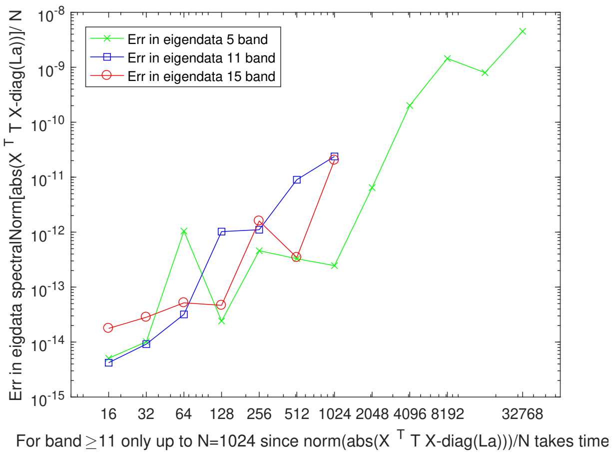

FIG. 6.4. *Here we test at once all the eigendata of a Toeplitz matrix T by computing the spectral norm of the matrix containing the absolute values of the entries of the matrix $X^TTX - D$, where the diagonal matrix D contains the eigenvalues of T and the columns of X are the corresponding normalized eigenvectors. We divided the results by the size N of the matrix.*

7. Conclusions. The method presented here is the method of choice for computing distinct eigenvalues of band symmetric Toeplitz matrices. As it is very fast, for instance on our computer the time for a 2-band matrix of size $2^{15} \times 2^{15}$ is 0.001 seconds, one can compute all the eigenvalues by this method. But if only a selected cluster of eigenvalues is wanted, then the method established in this paper would also find, due to interlacing properties, a quite small interval where these particular eigenvalues hide.

Due to the interlacing property of the eigenvalues of the perturbation matrix, for which we give an explicit formula, the lower and upper bound for each eigenvalue can be used, together with the ones in [2] and the ones which have been obtained by using the circulant matrix associated to a band Toeplitz matrix, in order to better approximate the eigenvalues that we seek.

The function which finds the number ν of eigenvalues that are less than a given real number λ needs, for a $2q+1$-diagonals Toeplitz matrix T_q, only less than $(3q^2 - q + 2.5)N$ arithmetical operations (including comparisons but not including the loop counter), and the optimized version for $q = 2$ needs only $9.5N$ operations. This is important, since this function is used many times in the process of bisection, and one can see that for a pentadiagonal matrix, the complexity is only twice larger than that of the classic one from the paper [1] for tridiagonal matrices.

The algorithm for finding eigenvectors works only for eigenvalues of multiplicity one, for instance, for any eigenvalue of a 2-band symmetric Toeplitz matrix. This algorithm, which appeared in [11], has not been much improved in this paper, except that here we compute only half of each eigenvector due to the fact that the eigenvectors are either symmetric or skew-symmetric. This diminishes the error and so does the fact that most of the entries of the quasiseparable generators, with which we multiply frequently, are equal to 0 and 1. To our surprise, the orthogonality of the eigenvectors is kept even for 7-band matrices (with 15 diagonals) of size 8192×8192. Moreover, the eigenvectors are obtained at a very low complexity cost.

Acknowledgments. The authors are very grateful to Michiel Hochstenbach for his deep involvement and his very important contribution to the paper with both time and expertise.

Appendix A. Yet a faster algorithm especially for 2-band matrices.

In this special case, the algorithm receives as input the size N of the 2-band symmetric Toeplitz matrix T_2 and its 3 Toeplitz coefficients, namely the diagonal entry $d \equiv t_0$ and a size-2 vector $q = (t_1, t_2)$, where $t_2 > 0$. It computes the eigenvalues $\lambda(1 : N)$ of the perturbed matrix A_2, where

$$A_2(i,j) = T_2(i,j), \qquad i,j = 1,\dots,N, \quad i+j \neq 2, i+j \neq 2N \quad \text{and}$$
$$A(N,N) = A(1,1) = T(1,1) - t_2.$$

A.1. Find the number ν of sign changes in the Sturm sequence for a 2-band matrix. The procedure to find the number ν of sign changes in the Sturm sequence presented in Algorithm 5.1 reads as follows for a 2-band matrix.

ALGORITHM A.1 (**Find ν**).
The number ν of sign changes in the Sturm sequence for a given real value λ and for an $N \times N$ 2-band symmetric Toeplitz matrix T_2, with a given diagonal entry $d \equiv t_0$ and given Toeplitz coefficients $s = t_1, r = t_2$, is computed by the following steps.

1. Compute $\delta = d - \lambda$, $u_1 = \begin{bmatrix} s/\delta & r/\delta \end{bmatrix}^T$, $f_1 = u_1 \begin{bmatrix} s & r \end{bmatrix}$.
   Set $\nu = 1$ if $\delta < 0$ and $\nu = 0$ otherwise.
2. For $k = 2, \dots, N-1$ compute

$$\phi_k = \begin{bmatrix} s - f_{k-1}(2,1) \\ r \end{bmatrix}, \quad D_k = \delta - f_{k-1}(1,1), \quad u_k = \phi_k / D_k,$$
$$f_k = \begin{bmatrix} f_{k-1}(2,2) & 0 \\ 0 & 0 \end{bmatrix} + u_k \phi_k^T.$$

   Set $\nu = \nu + 1$ if $D_k < 0$.
3. Set $\nu = \nu + 1$ if $\delta - f_{N-1}(1,1) < 0$.

In the optimized form one obtains the following version:

ALGORITHM A.2 (**Find ν**).
The number ν of sign changes in the Sturm sequence for a given real value λ and for an $N \times N$ 2-band symmetric Toeplitz matrix T_2, with the given diagonal entry $d \equiv t_0$ and the given Toeplitz coefficients $q = t_1, r = t_2$, is computed by the following steps.

1. Compute $\delta = d - \lambda$, $s = r^2$, $f = q^2/\delta$, $g = qr/\delta$, $h = s/\delta$, and set $\nu = 1$ if $\delta < 0$ and $\nu = 0$ otherwise.
2. Compute $N - 2$ times $D = \delta - f$, $u = q - g$, $f = h + u^2/D$, $g = ur/D$, $h = s/D$, and set each time $\nu = \nu + 1$ if $D < 0$.
3. Set $\nu = \nu + 1$ if $\delta - f < 0$.

This algorithm is an optimized version of Algorithm A.1, in which f, g, h are in fact $f(1,1)$, $f(2,1)$, $f(2,2)$, respectively.

The complexity of the above algorithm is less than $9.5N$ arithmetical operations, where assignments and the loop counter have not been counted. Moreover, it uses no matrices or indices, so it is very fast indeed. We point out that the complexity is not much higher than the complexity of the similar function for tridiagonal symmetric matrices introduced and used in [27] and [1].

A.2. Consecutive eigenvalues of the perturbed matrix which remain consecutive after ordering them all in increasing order. In the general case, the eigenvalues of the perturbed matrix A_2 of a 2-band Toeplitz matrix decrease to a minimum and then increase. But if $|t_1| \geq 4t_2 \cos\left(\frac{\pi}{N+1}\right)$, for instance, then they are monotonous from the beginning.

We will show that in many cases consecutive eigenvalues of A_2 remain consecutive after ordering them. We will call this the **C**-property. (Extensive numerical experiments suggest that in this case, when no other eigenvalue of A_2 interferes, the corresponding eigenvalue of T_2 completely interlaces with them, i.e.,

$$\lambda_k^A \le \lambda_k^T \le \lambda_{k+1}^A, \tag{A.1}$$

or vice versa. However, we cannot prove (A.1) under the above condition so we do not claim it.)

In the following theorem $\lfloor z \rfloor$ denotes the largest integer less than or equal to the real number z.

THEOREM A.3 (2-band interlacing). *Let T_2 be a 2-band symmetric Toeplitz matrix of size $N \times N$ with Toeplitz coefficients t_0, t_1 on the diagonal and, respectively, the first sub-diagonals and t_2 on the second sub-diagonals. Without loss of generality one can assume $t_2 > 0$. Let A_2 be its perturbed matrix such that*

$$\begin{aligned} A_2(i,j) &= T_2(i,j), \qquad\qquad i,j = 1,\dots,N, 2 < i+j < 2N,\\ A_2(N,N) = A_2(1,1) &= T_2(1,1) - t_2. \end{aligned}$$

Denote

$$p = \frac{t_1}{4t_2}, \qquad \alpha = \frac{\pi}{N+1}, \qquad m = \left\lfloor \frac{\arccos(-p)}{\alpha} + 0.5 \right\rfloor. \tag{A.2}$$

Then sufficient conditions under which the eigenvalues of A_2,

$$\lambda_k^A = t_0 + 2t_1 \cos(k\alpha) + 2t_2 \cos(2k\alpha), \qquad k = 1,\dots,N, \tag{A.3}$$

have the **C***-property are as follows.*

1) *If $p \le -1$, then the eigenvalues in (A.3) are already sorted in ascending order upon k.*
2) *If $p \ge 1$, then the eigenvalues in (A.3) are already sorted in descending order upon k.*
3) *If $-1 < p < 0$ and*

$$s = \left\lfloor \frac{\arccos(-p - |p + \cos(\alpha)|)}{\alpha} + 0.5 \right\rfloor, \tag{A.4}$$

then the eigenvalues in (A.3) are sorted in descending order upon k, for $k = 1,\dots,m$, (with m from (A.2)) and in ascending order upon k, for $k = m,\dots,N$, and for

$$k = s, s+1, \dots, N-1, \qquad \text{or} \qquad k = 2j,\ j = 1,2,\dots,\left\lfloor \frac{s-1}{2} \right\rfloor, \tag{A.5}$$

$\lambda_k^A < \lambda_{k+1}^A$ have the **C** *property. In particular if $p \le -\cos(\alpha)$ then A_2 satisfies in this case condition 3).*

4) *If $0 < p < 1$ and*

$$s = \left\lfloor N + 1 - \frac{\arccos(-p + |p - \cos(\alpha)|)}{\alpha} + 0.5 \right\rfloor, \tag{A.6}$$

then the eigenvalues in (A.3) are sorted in ascending order upon k, for $k = 1,\dots,m$, and in descending order upon k, for $k = m,\dots,N$, and after sorting all the eigenvalues of A_2 in ascending order, formula (A.5) holds but now with the s given by (A.6). In particular if $p \ge \cos(\alpha)$, then A_2 satisfies in this case condition 4).

ETNA
Kent State University and
Johann Radon Institute (RICAM)

5) If $p = 0$, then after sorting all the eigenvalues of A_2 in ascending order,

$$\lambda^A_{2j-1} = \lambda^A_{2j} \leq \lambda^T_{2j-1} < \lambda^T_{2j} \leq \lambda^A_{2j+1} = \lambda^A_{2j+2}, \qquad j = 1, 2, \ldots, \frac{N-2}{2}$$

if N is even. If N is odd and $r = \frac{N+1}{2}$, then before sorting, for the eigenvalues of A_2, λ^A_r is the only minimal eigenvalue of A_2 while the other eigenvalues satisfy $\lambda^A_{r-j} = \lambda^A_{r+j}$, $j = 1, 2, \ldots, r-1$.

Proof. If we denote

$$x_k = \cos\left(\frac{k\pi}{N+1}\right),$$

then the corresponding eigenvalue λ^A_k, by using the formula of the cosine of a double angle, will be $\lambda(k) = t_0 + 2t_1x_k + 2t_2(2x_k^2 - 1)$, which is one of the points on the parabola $4t_2x^2 + 2t_1x + t_0 - 2t_2$ that has a minimum at $x_0 = -\frac{t_1}{4t_2} = -p$.

Consider the function $f : [1, N] \to \mathbb{R}$ defined by

$$f(u) = t_0 + 2t_1 \cos\left(\frac{u\pi}{N+1}\right) + 2t_2 \cos\left(\frac{2u\pi}{N+1}\right).$$

Then $f(u) = g(h(u))$, where

$$h : [1, N] \to \mathbb{R}, \quad h(u) = \cos\left(\frac{u\pi}{N+1}\right) \qquad \text{and}$$
$$g : [-1, 1] \to \mathbb{R}, \quad g(x) = 4t_2x^2 + 2t_1x + t_0 - 2t_2.$$

The derivative of f is $f'(u) = g'(h(u))h'(u)$, but $h'(u) < 0$ on the interval $[1, N]$ since then the argument of the cosine belongs to the interval $(0, \pi)$ and only $g'(x)$ can be zero. Since the graph of g is a parabola, a minimum can occur only at its middle point $\frac{-t_1}{4t_2}$.

If we denote $p = \frac{t_1}{4t_2}$, then, if $p < -1$ or $p > 1$, the function g also has no extremum in the desired interval.

If the minimum $x_0 \in (-1, 1)$, i.e., possibly between two cosines, then we consider the natural number m that is approximated by $\frac{N+1}{\pi} \arccos\left(-\frac{t_1}{4t_2}\right)$, and we advance leftwards and rightwards in computing in linear time the increasing sequence of the eigenvalues of A_2. We only have to compare the next λ^A_k from the left with the one from the right and each time we have to pick the smallest. When we have to advance both leftwards and rightwards starting with the minimum, in order to build the increasing sequence of the eigenvalues of A_2, it might be that an eigenvalue of A_2 from the left-hand side, or vice versa, interferes between the eigenvalue λ^A_k from the right-hand side and its corresponding eigenvalue λ^T_k of T_2, but otherwise the eigenvalues of A_2 are monotonic, thus they have the **C** property.

Case 1) If $p < -1$, then $t_1 \leq -4t_2$, and the minimum of the parabola is before -1, and then the eigenvalues of A_2 are already sorted in ascending order.

Case 2) If $p \geq 1$, i.e., $t_1 \geq 4t_2$, then the minimum of the parabola is larger than 1, thus the eigenvalues of A_2 are already sorted in descending order, and their order simply has to be reversed.

Case 3)–4.) When $-1 < p < 1$, the minimum is in the range of the cosines, and we have to advance both leftwards and rightwards starting with the minimum, in order to build the increasing sequence of the eigenvalues of A_2. Then it might be that one of the branches stops. Afterwards, only one branch remains, and the eigenvalues of A_2, which follow after

ETNA
Kent State University and
Johann Radon Institute (RICAM)

that point on, are already sorted in order, and none of them can still interfere between a certain eigenvalue λ_k^A and its next one.

If $-1 < p < 0$, in case 3), then the left branch finishes earlier since its stopping point for $k = 1$ is below the stopping point for $k = N$ of the right branch. The finishing values are, before sorting all the eigenvalues of A_2 in ascending order according to (A.3),

$$\begin{aligned} \lambda_1^A &= t_0 + 2t_1 \cos(\alpha) + 2t_2 \cos(2\alpha), \\ \lambda_N^A &= t_0 + 2t_1 \cos(N\alpha) + 2t_2 \cos(2N\alpha). \end{aligned} \tag{A.7}$$

Taking into account that

$$\cos(N\alpha) = -\cos(\alpha)$$

for α as given in (A.2) and that $\cos(2N\alpha) = \cos(2\alpha)$, the number from (A.7) becomes

$$\lambda_N^A = t_0 - 2t_1 \cos(\alpha) + 2t_2 \cos(2\alpha), \tag{A.8}$$

which for negative t_1, i.e., negative p, is larger than λ_1^A, as $0 < \alpha < \frac{\pi}{2}$.

Regarding the expression $f(u) = t_0 + 2t_1 \cos(u\alpha) + 2t_2 \cos(2u\alpha)$ as a continuous function, we want to find for which u_0 we have $f(u_0) = \lambda_1^A$, in order to find where from the right branch remains the only one. We claim that the natural number which approximates u_0 is s from (A.4). Indeed, if we denote $x = \cos(u\alpha)$, and we use the formula for the cosine of the double angle as being $2x^2 - 1$. Thus, we must solve the equation

$$4t_2x^2 + 2t_1x + t_0 - 2t_2 = \lambda_1^A,$$

which, after dividing by $4t_2$ and denoting $M = \frac{\lambda_1^A - t_0}{4t_2}$ becomes

$$x^2 + 2px - 0.5 = M. \tag{A.9}$$

Its discriminant divided by 4 is

$$\begin{aligned} \Delta &= p^2 + 0.5 + M = p^2 + 0.5 + \frac{2t_1 \cos(\alpha) + 2t_2 \cos(2\alpha)}{4t_2} \\ &= p^2 + 0.5 + 2p\cos(\alpha) + 0.5\cos(2\alpha), \end{aligned}$$

which after using that $0.5(1 + \cos(2\alpha)) = \cos^2(\alpha)$ becomes $\Delta = (p + \cos(\alpha))^2$. Therefore, its square root is $|p + \cos(\alpha)|$ and (A.4) readily follows from (A.9). Indeed, $x = \cos(u\alpha)$, so that, if we found x, we must use $\arccos(x)$ and divide the result by α.

If $p \le -\cos(\alpha)$, then the absolute value is that of a negative number, and p from (A.4) simplifies, and we obtain $\frac{\arccos(\cos(\alpha))}{\alpha} + 0.5$, which is equal to 1.5 and its integer value is 1, so that starting from 1 on, only one branch remains, which means for our problem that after sorting the eigenvalues of A_2 in ascending order, the **C**-property occurs.

4) Due to formula (A.8), we obtain s from (A.6) in a similar way. Note that now the other root of (A.9) is the one for the left branch.

If $p \ge \cos(\alpha)$, then the absolute value from (A.6) is of a positive number, and p from equation (A.6) simplifies, and we obtain $N + 1 - \frac{\arccos(-\cos(\alpha))}{\alpha} + 0.5$, which is equal to $N + 1.5 - \frac{\pi - \alpha}{\alpha} = N + 1.5 - N$, and its integer value is 1, so that starting from 1 on, only the left branch remains, which means for our problem that, after sorting the eigenvalues of A_2 in ascending order, the **C**-property occurs.

5) If $p = 0$, i.e., $t_1 = 0$, then by (A.7) and (A.8) both branches end at the same level. Moreover, before sorting the eigenvalues of A_2 in ascending order, we have

$$\lambda_k^A = \lambda_{N-k}^A, \qquad k = 1, \ldots, \left\lfloor \frac{N}{2} \right\rfloor. \qquad \square$$

COROLLARY A.4. *The eigenvalues λ_k^A, $k = 1, 2, \ldots, N$, of A_2 are already ordered upon k if and only if*

$$|t_1| \geq 4 \cos\left(\frac{\pi}{4(N+1)}\right) \cos\left(\frac{3\pi}{4(N+1)}\right) t_2. \tag{A.10}$$

They are increasing or decreasing, according to whether the sign of t_1 is minus or plus, respectively.

Proof. With the definitions in (A.2), the inequality (A.10) becomes

$$|p| \geq \cos\left(\frac{\alpha}{4}\right) \cos\left(\frac{3\alpha}{4}\right). \tag{A.11}$$

If $p < 0$, then we know from case 3) of the preceding theorem that the eigenvalues of A_2 are ascending if $p \leq -\cos(\alpha)$. So this remains to be proved for $-\cos(\alpha) < p < 0$. In this case, the absolute value in (A.4) is that of a positive number, therefore s is at most 1 if and only if

$$\frac{\arccos\left(-2p - \cos(\alpha)\right)}{\alpha} + 0.5 \leq 1,$$

which is equivalent to $\arccos\left(-2p - \cos(\alpha)\right) \leq 0.5\alpha$.

Since $0.5\alpha < \pi$, we can apply the decreasing function cosine to both sides, and then we obtain $-2p - \cos(\alpha) \geq \cos(0.5\alpha)$, which is equivalent to

$$p \leq -\frac{1}{2}(\cos(0.5\alpha) + \cos(\alpha)),$$

which gives (A.11) for negative p.

If $p > 0$, then we know from case 4) of the preceding theorem that the eigenvalues of A_2 are descending if $p \geq \cos(\alpha)$. So this remains to be proved for $0 < p < \cos(\alpha)$. In this case, the absolute value in (A.6) is that of a negative number. Therefore s is at most 1 if and only if

$$N + 1 - \frac{\arccos\left(-2p + \cos(\alpha)\right)}{\alpha} \leq 1 - 0.5,$$

which is equivalent to $\arccos\left(-2p + \cos(\alpha)\right) \geq \alpha(N + 0.5)$.

Since $\alpha(N + 0.5) < (N + 1)\alpha = \pi$, we can apply the decreasing function cosine to both sides, and then we obtain $-2p \leq \cos\left(\frac{(N+0.5)\pi}{N+1}\right) - \cos(\alpha)$, which is equivalent again to (A.11), since $\cos\left(\frac{2N+1}{2}\alpha\right) = \cos\left(\frac{(2N+2)\pi}{2(N+1)} - \frac{\alpha}{2}\right) = \cos\left(\pi - \frac{\alpha}{2}\right) = -\cos\left(\frac{\alpha}{2}\right)$, and if $-2p \leq -\cos\left(\frac{\alpha}{2}\right) - \cos(\alpha)$, then $|p| = p \geq \frac{1}{2}(\cos(0.5\alpha) + \cos(\alpha))$. $\square$

A.3. Complete and faster algorithm for the eigenvalues of 2-band symmetric Toeplitz matrices.

ALGORITHM A.5.

The eigenvalues and the eigenvectors for an $N \times N$ 2-band symmetric Toeplitz matrix T_2, with a given diagonal entry $d \equiv t_0$ and given Toeplitz coefficients $q = t_1, r = t_2$, are computed by the following steps.

ETNA
Kent State University and
Johann Radon Institute (RICAM)

1. Find a lower and an upper overall bound, say B_L and B_U, respectively, for all the eigenvalues of T_2 such as in Section 4.1. For instance, compute the Gershgorin bounds (4.2) $t_0 - |t_1| - t_2$ and $t_0 + |t_1| + t_2$ or compute the Frobenius norm F of T_2. Formula (4.1) now becomes

$$F = \sqrt{N t_0^2 + 2(N-1)t_1^2 + 2(N-2)t_2^2}.$$

2. Scale the matrix by dividing its 3 Toeplitz coefficients by F. This will make all the eigenvalues sub-unitary and will prevent overflow.
   Set a variable $\sigma = 1$.
   If $t_2 < 0$, then change the signs for all the three Toeplitz coefficients, and set $\sigma = -1$, and at the end change back the sign of the N found eigenvalues.
3. Find the eigenvalues $\lambda_A(1), \ldots, \lambda_A(N)$ of the perturbed matrix A_2 by the formula

$$\lambda_A(k) = t_0 + 2t_1 \cos\left(\frac{k\pi}{N+1}\right) + 2t_2 \cos\left(\frac{2k\pi}{N+1}\right), \quad k = 1, 2, \ldots, N.$$

4. Sort the eigenvalues which have been obtained in the previous step in ascending order. Note that in many cases, for instance, if $|t_1| > 4t_2$, they are sorted already, and if one cannot start from the minimal eigenvalue and advance leftwards and rightwards, then one can decide from only one comparison which eigenvalue is lower. Denote the sorted eigenvalues again by $\lambda_A(1:N)$ and build as follows all the possible limits $B(k)$, $k = 1, \ldots N+1$, of the bounding intervals which are supposed to contain the eigenvalues of T_2, namely

$$B(1:N) = \lambda_A(1:N), \quad B(N+1) = 1. \tag{A.12}$$

5. Find specific lower and upper bounds for each and every eigenvalue of T_2. For this perform steps 5.1 and 5.2.
   5.1. Set $\nu(N+1) = N$, $\nu(1) = 0$, $L_0(N+1) = 1$.
   5.2. For $k = 1, \ldots, N$, find $\nu(k+1)$ with Algorithm A.2 for the real number $\lambda = B(k+1)$, where B is the array from (A.12). In fact, for $k = N$, we already had the result in step 5.1., and if k is odd or if it is larger than s, from (A.4) or (A.6), whichever applies, then $\nu(k) = k - 1$. However, for about a quarter of the values of k, the function which finds ν must be used.
   Compute the index

$$i = 2k - \nu(k+1), \tag{A.13}$$

   and set the lower and the upper bound for the kth eigenvalue as $L_0(k) = B(i)$ and $U_0(k) = B(i+1)$.
6. 6.1. Set a value $\varepsilon = 2\varepsilon_0$, where ε_0 is the machine precision.
   Set $f = 0$ if this is the number of already found or unnecessary smaller eigenvalues.
   6.2. For $k = 1, \ldots, N$ perform all three steps 6.2.1, 6.2.2, and 6.2.3.
      6.2.1. If $L_0(k) = L_0(k+1)$ perform the following
      while loop as long as $U_0(k) - L_0(k) > \varepsilon$.
      Set $\lambda = (L_0(k) + U_0(k))/2$ and find ν with Algorithm A.2 for the real number λ.
      If $\nu = f$ set $L_0(k) = \lambda$
      else

ETNA
Kent State University and
Johann Radon Institute (RICAM)

if $\nu = f + 2$ set $U_0(k+1) = \lambda$
else
set $U_0(k) = L_0(k+1) = \lambda$ and break the *while* loop.

6.2.2. Even if we performed the previous step 6.2.1., if $L_0(k)$ does not equal $L_0(k+1)$, perform the following
while loop as long as $U_0(k) - L_0(k) > \varepsilon$.
Set $\lambda = (L_0(k) + U_0(k))/2$ and find ν with Algorithm A.2 for the real number λ.
If $\nu = f$ set $L_0(k) = \lambda$
else
set $U_0(k) = \lambda$.

6.2.3. Set $\lambda_T(k) = (L_0(k) + U_0(k))/2$ and make $f = f + 1$.

7. De-scale the eigenvalues by multiplying them with σF as computed in step 1.

Proof. We will show that formula (A.13) is correct. For $k = 1$, if $\nu(2) = 1$, then the first eigenvalue is in the interval $[\lambda_1^A, \lambda_2^A]$ so that $i = 1$, which is indeed $2k - \nu(2)$. If, on the contrary, $\nu(2) = 0$, then the first eigenvalue is in the interval $[\lambda_2^A, \lambda_3^A]$ so that $i = 2$, which is indeed $2k - \nu(2)$, exactly what (A.13) claims. Suppose now that formula (A.13) is true for a certain k. Then, for $k + 1$, there are three possibilities for $\nu(k+2)$: it can be larger than $\nu(k+1)$ by $0, 1$ or 2. An examination of each case proves the induction step for the considered formula. ∎

A.4. Find the normalized eigenvector for an already found eigenvalue λ of a 2-band matrix. All the eigenvalues of such a matrix have multiplicity one.

ALGORITHM A.6.
The eigenvector for a given eigenvalue λ and for an $N \times N$ 2-band symmetric Toeplitz matrix T_2, with the given diagonal entry $d \equiv t_0$ and the given Toeplitz coefficients $q = t_1, r = t_2$, is computed by the following steps.

1. 1.1. Compute

$$\delta = d - \lambda, \qquad u(1) = q/\delta, \qquad v(1) = r/\delta, \qquad \text{and}$$
$$f = qu(1), \qquad g = qv(1), \qquad h = v(1)r.$$

1.2. For $k = 2, \ldots, N-1$ compute

$$D = \delta - f, \qquad v(k) = r/D, \qquad u(k) = (q-g)/D,$$
$$f = h + (u(k))^2 D, \qquad g = u(k)v(k)D, \qquad h = (v(k))^2 D.$$

1.3. Set $x(N) = 1, s_1 = 1, s_2 = 0$.

2. 2.1. For $k = N-1, \ldots, 2$ compute

$$x(k) = -u(k)s_1 - v(k)s_2, \qquad s_2 = s_1, \qquad s_1 = x(k).$$

2.2. Compute $x(1) = -u(1)s_1 - v(1)s_2$ and normalize the vector x by dividing it by its norm n, which is computed fast by

$$n = \sqrt{2 \sum_{k=1}^{(N-\rho)/2} (x(k))^2 + \rho \left(x\left(\frac{N+\rho}{2}\right)\right)^2},$$

where ρ is the reminder of the integer division of N by 2.

Proof. This algorithm is a particular case of the Algorithm 5.5, in which u and v are one-dimensional vectors of size $N-1$, which appear instead of the first and second coordinate of the multidimensional u from that algorithm and where f, g, h are in fact $f(1,1)$, $f(2,1)$, $f(2,2)$, respectively. Also, we have now used the fact that the eigenvector is either symmetric or skew-symmetric. ∎

The complexity of the above algorithm is less than $14N$ arithmetical operations, where assignments and loop counters have not been counted and also not the computation of the norm n of the eigenvector. Moreover, this algorithm uses only three vectors with indices so that it is very fast indeed.

REFERENCES

[1] W. BARTH, R. S. MARTIN, AND J. H. WILKINSON, *Calculations of the eigenvalues of a symmetric tridiagonal matrix by the method of bisection*, Numer. Math., 9 (1967), pp. 386–393.

[2] D. BINI AND M. CAPOVANI, *Spectral and computational properties of band symmetric Toeplitz matrices*, Linear Algebra Appl., 52/53 (1983), pp. 99–126.

[3] D. BINI AND V. PAN, *On the evaluation of the eigenvalues of banded block Toeplitz block matrices*, J. Complexity, 7 (1991), pp. 408–424.

[4] ———, *Polynomial and Matrix Computations. Vol I.*, Birkhäuser, Boston, 1994.

[5] A. CANTONI AND P. BUTLER, *Eigenvalues and eigenvectors of symmetric centrosymmetric matrices*, Linear Algebra Appl., 13 (1976), pp. 275–288.

[6] Y. EIDELMAN AND I. GOHBERG, *On a new class of structured matrices*, Integral Equations Operator Theory, 34 (1999), pp. 293–324.

[7] Y. EIDELMAN, I. GOHBERG, AND I. HAIMOVICI, *Separable Type Representations of Matrices and Fast Algorithms. Vol. 1*, Oper. Theory Adv. Appl. 234, Birkhäuser, Basel, 2014.

[8] ———, *Separable Type Representations of Matrices and Fast Algorithms. Vol. 2.*, Oper. Theory Adv. Appl. 235, Birkhäuser, Basel, 2014.

[9] Y. EIDELMAN, I. GOHBERG, AND V. OLSHEVSKY, *Eigenstructure of order-one-quasiseparable matrices. Three-term and two-term recurrence relations*, Linear Algebra Appl., 405 (2005), pp. 1–40.

[10] Y. EIDELMAN AND I. HAIMOVICI, *The fast bisection eigenvalue method for Hermitian order one quasiseparable matrices and computations of norms*, Electron. Trans. Numer. Anal., 44 (2015), pp. 342–366. https://etna.ricam.oeaw.ac.at/vol.44.2015/pp342-366.dir/pp342-366.pdf

[11] ———, *Bisection eigenvalue method for Hermitian matrices with quasiseparable representation and a related inverse problem*, in Operator Theory, Analysis and the State Space Approach, H. Bart, S. ter Horst, A. C. M. Ran, and H. J. Woerdeman, eds., vol. 271 of Oper. Theory Adv. Appl., Birkhäuser/Springer, Cham, 2018, pp. 181–200.

[12] S. E. EKSTRÖM, C. GARONI, AND S. SERRA CAPIZZANO, *Are the eigenvalues of banded symmetric Toeplitz matrices known in almost closed form?*, Exp. Math., 27 (2018), pp. 478–487.

[13] S.-E. EKSTRÖM AND S. SERRA-CAPIZZANO, *Eigenvalues and eigenvectors of banded Toeplitz matrices and the related symbols*, Numer. Linear Algebra Appl., 25 (2018), Paper No. e2137, 17 pages.

[14] D. J. EVANS, *A recursive algorithm for determining the eigenvalues of a quindiagonal matrix*, Comput. J., 18 (1975), pp. 70–73.

[15] G. H. GOLUB AND C. F. V. LOAN, *Matrix Computations*, 4th ed., Johns Hopkins University Press, Baltimore, 2013.

[16] A. J. HOFFMAN AND H. W. WIELANDT, *The variation of the spectrum of a normal matrix*, Duke Math. J., 20 (1953), pp. 37–39.

[17] A. HORN, *Eigenvalues of sums of Hermitian matrices*, Pacific J. Math., 12 (1962), pp. 225–241.

[18] R. A. HORN AND C. R. JOHNSON, *Matrix Analysis*, 2nd ed., Cambridge University Press, Cambridge, 2013.

[19] G. D. SMITH, *Numerical Solution of Partial Differential Equations*, 2nd ed., Oxford University Press, New York, 1978.

[20] J. STOER AND R. BULIRSCH, *Introduction to Numerical Analysis*, 3rd ed., Springer, New York, 2002.

[21] W. A. SENTANCE AND I. P. CLIFF, *The determination of eigenvalues of symmetric quindiagonal matrices*, Comput. J., 24 (1981), pp. 177–179.

[22] S. SERRA CAPIZZANO AND D. SESANA, *A note on the eigenvalues of g-circulants (and of g-Toeplitz, g-Hankel matrices)*, Calcolo, 51 (2014), pp. 639–659.

[23] W. F. TRENCH, *On the eigenvalue problem for Toeplitz band matrices*, Linear Algebra Appl., 64 (1985), pp. 199–214.

[24] R. VANDEBRIL, M. VAN BAREL, AND N. MASTRONARDI, *Matrix Computations and Semiseparable Matrices. Vol. I*, Johns Hopkins University Press, Baltimore, 2008.

ETNA
Kent State University and
Johann Radon Institute (RICAM)

[25] ———, *Matrix Computations and Semiseparable Matrices. Vol. II*, Johns Hopkins University Press, Baltimore, 2008.
[26] H. WEYL, *Das asymptotische Verteilungsgesetz der Eigenwerte linearer partieller Differentialgleichungen (mit einer Anwendung auf die Theorie der Hohlraumstrahlung)*, Math. Ann., 71 (1912), pp. 441–479.
[27] J. H. WILKINSON, *Calculation of the eigenvalue of a symmetric tridiagonal matrix by the method of bisection*, Numer. Math., 4 (1962), pp. 362–367.
[28] ———, *The Algebraic Eigenvalue Problem*, Claredon Press, Oxford, 1965.