Numerical solution of the inverse eigenvalue problem for real symmetric Toeplitz matrices

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NUMERICAL SOLUTION OF THE INVERSE EIGENVALUE PROBLEM FOR REAL SYMMETRIC TOEPLITZ MATRICES

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Abstract. H.J. Landau has recently given a nonconstructive proof of an existence theorem for the inverse eigenvalue problem for real symmetric Toeplitz (RST) matrices. This paper presents a procedure for the numerical solution of this problem. The procedure is based on an implementation of Newton’s method that exploits Landau’s theorem and other special spectral properties of RST matrices. With this version of Newton’s method, together with the strategy proposed for applying it, the method appears to be globally convergent; however, this is not proved.

Key words. eigenvalue, eigenvector, Newton’s method, Toeplitz matrix

AMS subject classifications. 15A18, 15A42

1. Introduction. Let \( t = [t_0\ t_1\ \cdots\ t_{n-1}] \) where \( t_0, t_1, \ldots, t_{n-1} \) are real numbers, and let \( T(t) \) be the real symmetric Toeplitz (RST) matrix
\[
T(t) = (t_{i-j})_{i,j=1}^n.
\]
We say that \( t \) generates \( T(t) \). We denote the eigenvalues of \( T(t) \) by
\[
\lambda_1(t) \leq \lambda_2(t) \leq \cdots \leq \lambda_n(t).
\]

The inverse eigenvalue problem for RST matrices is as follows.

**Problem 1.** Given \( n \) real numbers \( \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n \), find an \( n \)-vector \( \hat{t} \) such that \( \lambda_i(\hat{t}) = \hat{\lambda}_i, \quad 1 \leq i \leq n \).

We will call \( \lambda_1, \lambda_2, \ldots, \lambda_n \) the target eigenvalues and \( \hat{\lambda} = [\hat{\lambda}_1\ \hat{\lambda}_2\ \cdots\ \hat{\lambda}_n] \) the target spectrum.

Problem 1 is a special case of an inverse eigenvalue problem for symmetric matrices considered by Friedland, Nocedal, and Overton [5]. We present a numerical method for solving Problem 1.

2. Normalization. If \( t = [t_0\ t_1\ \cdots\ t_{n-1}] \) then the trace of \( T(t) \) equals \( nt_0 \); therefore, if \( \hat{t} \) is a solution of Problem 1 then
\[
\hat{t}_0 = \frac{\hat{\lambda}_1 + \hat{\lambda}_2 + \cdots + \hat{\lambda}_n}{n}.
\]
If \( \hat{\lambda}_1 = \hat{\lambda}_2 = \cdots = \hat{\lambda}_n = \hat{\lambda} \) then \( \hat{t} = [\hat{\lambda} \ 0 \ \cdots \ 0] \) is a solution of Problem 1; therefore we assume that the target eigenvalues are not all equal. For computational purposes it is convenient to assume that the target spectrum is normalized so that
\[
\hat{\lambda}_1 + \hat{\lambda}_2 + \cdots + \hat{\lambda}_n = 0
\]
(2) \[ \hat{\lambda}_1^2 + \hat{\lambda}_2^2 + \cdots + \hat{\lambda}_n^2 = 1. \]

This implies no loss of generality, since if either (1) or (2) does not hold, we can introduce the new target eigenvalues \( \hat{\lambda}_1, \hat{\lambda}_2, \ldots, \hat{\lambda}_n \) defined by

\[ \hat{\lambda}_i = \frac{\hat{\lambda}_i - \hat{t}_0}{S}, \quad 1 \leq i \leq n, \]

where

\[ S = \left( \sum_{i=1}^{n} (\hat{\lambda}_i - \hat{t}_0)^2 \right)^{1/2}. \]

These modified target eigenvalues satisfy conditions analogous to (1) and (2). A solution of Problem 1 for the modified spectrum must be of the form \( \hat{t} = [0 \hat{t}_1 \cdots \hat{t}_{n-1}] \), and \( t = [\hat{t}_0 \hat{S} \hat{t}_1 \cdots \hat{S} \hat{t}_{n-1}] \) is a solution of the original problem.

3. Laurie’s algorithm. Laurie [8] has proposed an algorithm for solving Problem 1. In order to state this algorithm, suppose that \( T(t) \) has distinct eigenvalues \( \lambda_1(t) < \lambda_2(t) < \cdots < \lambda_n(t) \) with associated unit eigenvectors \( p_i(t) = [p_{i1}(t) p_{i2}(t) \cdots p_{in}(t)]^T \), \( 1 \leq i \leq n \).

(The ambiguity in the direction of \( p_i(t) \) is not important.) Laurie’s algorithm obtains \( \hat{t} \) as the limit of a sequence \( \{t_m\}_{m=0}^{\infty} \), where \( t^0 \) is chosen arbitrarily and

\[ p_i(t_m^{-1})^T T(t_m) p_i(t_m^{-1}) = \hat{\lambda}_i, \quad 1 \leq i \leq n. \]

(Laurie also suggested a variation of this implementation, which we will discuss in §6.) Thus, the Rayleigh quotients of \( T(t_m) \) with respect to the eigenvectors of \( T(t_m^{-1}) \) are equal to the respective target eigenvalues. For this reason Laurie called this method “the reverse Rayleigh quotient algorithm.” However, (3) can be written as

\[ \sum_{k=1}^{n} c_{ik}(t_m^{-1}) t_{k-1}^m = \hat{\lambda}_i, \quad 1 \leq i \leq n, \]

where

\[ c_{i1}(t_m^{-1}) = 1, \]

\[ c_{ik}(t_m^{-1}) = 2 \sum_{l=1}^{n-k+1} p_{il}(t_m^{-1}) p_{i,l+k-1}(t_m^{-1}), \quad 2 \leq k \leq n, \quad 1 \leq i \leq n, \]

and it can be shown by specializing the arguments of Friedland, Nocedal, and Overton [5] that

\[ c_{ik}(t_m^{-1}) = \frac{\partial \lambda_i}{\partial t_{k-1}}(t_m^{-1}), \quad 1 \leq i, k \leq n. \]

Therefore the matrix of (4) is the Jacobian matrix of \( \lambda_1(t_m^{-1}), \lambda_2(t_m^{-1}), \ldots, \lambda_n(t_m^{-1}) \) with respect to \( t_0, t_1, \ldots, t_{n-1} \), which implies that Laurie’s algorithm is equivalent to Newton’s method, as Laurie acknowledged in a note added in proof to [8].
Laurie used the starting generator
\[ t^0 = [0 \ 1 \ 0 \ \cdots \ 0]. \]

He reported success in all computations in which he started with (5) and used full machine precision in diagonalizing the matrices \( \{T(t^m)\} \). However, since his algorithm is Newton's method, it is not globally convergent for the inverse eigenvalue problem. Moreover, it does not exploit the special spectral structure of RST matrices, or the current state of knowledge concerning the existence of a solution of Problem 1. We will review these matters in the next two sections.

4. Spectral properties of RST matrices. Following Andrew [1], we say that an \( n \)-vector \( x = [x_1 \ x_2 \ \cdots \ x_n]^T \) is symmetric if
\[ x_j = x_{n-j+1}, \quad 1 \leq j \leq n, \]
or skew–symmetric if
\[ x_j = -x_{n-j+1}, \quad 1 \leq j \leq n. \]
(Some authors call such vectors reciprocal and anti-reciprocal.)

Throughout this paper we let \( r = \lceil n/2 \rceil \) and \( s = \lfloor n/2 \rfloor \).

We now state four theorems that are special cases of results of Cantoni and Butler [2] for symmetric centrosymmetric matrices. As noted by Cantoni and Butler, these theorems imply that if \( T \) is an RST matrix of order \( n \) then \( R^n \) has an orthonormal basis consisting of \( r \) symmetric and \( s \) skew–symmetric eigenvectors of \( T \). They also lead to computational efficiency in our reformulation of Laurie's algorithm.

We will say that an eigenvalue \( \lambda \) of \( T \) is even (odd) if \( T \) has a symmetric (skew–symmetric) \( \lambda \)-eigenvector. In the following theorems \( J_m \) is the \( m \times m \) matrix with ones on the secondary diagonal and zeros elsewhere.

**Theorem 4.1.** Suppose that \( n = 2m \) and \( \mu \) is an eigenvalue of
\[ A = (t_{|i-j|} + t_{i+j-1})_{i,j=1}^m, \]
with associated unit eigenvector \( x \). Then \( \mu \) is an even eigenvalue of \( T \), with associated symmetric unit eigenvector
\[ p = \frac{1}{\sqrt{2}} \begin{bmatrix} J_m x \\ x \end{bmatrix}. \]

**Theorem 4.2.** Suppose that \( n = 2m \) and \( \nu \) is an eigenvalue of
\[ B = (t_{|i-j|} - t_{i+j-1})_{i,j=1}^m, \]
with associated unit eigenvector \( y \). Then \( \nu \) is an odd eigenvalue of \( T \), with associated skew-symmetric unit eigenvector
\[ q = \frac{1}{\sqrt{2}} \begin{bmatrix} -J_m y \\ y \end{bmatrix}. \]
Theorem 4.3. Suppose that $n = 2m + 1$ and $\mu$ is an eigenvalue of the matrix $A = (a_{ij})_{i,j=0}^{m}$ defined by

$$a_{ij} = \begin{cases} t_0 & \text{if } i = j = 0, \\ \sqrt{2}t_i & \text{if } j = 0, \\ \sqrt{2}t_j & \text{if } i = 0, \\ t_{|i-j|} + t_{i+j} & 1 \leq i, j \leq m, \end{cases}$$

with unit eigenvector $\begin{bmatrix} x_0 \\ x \end{bmatrix}$, where $x_0$ is a scalar. Then $\mu$ is an even eigenvalue of $T$, with associated symmetric unit eigenvector $p = \frac{1}{\sqrt{2}} \begin{bmatrix} J_m x \\ x_0 \sqrt{2} \\ x \end{bmatrix}$.

Theorem 4.4. Suppose that $n = 2m + 1$ and $\nu$ is an eigenvalue of $B = (t_{|i-j|} - t_{i+j})_{i,j=1}^{m}$, with associated unit eigenvector $y$. Then $\nu$ is an odd eigenvalue of $T$, with associated skew–symmetric unit eigenvector $p = \frac{1}{\sqrt{2}} \begin{bmatrix} -J_m y \\ 0 \\ y \end{bmatrix}$.

We will denote the even and odd eigenvalues of $T(t)$ by $\mu_1(t) \leq \mu_2(t) \leq \cdots \leq \mu_r(t)$ and $\nu_1(t) \leq \nu_2(t) \leq \cdots \leq \nu_s(t)$, respectively.

The last four theorems imply the following result.

Theorem 4.5. The even and odd eigenvalues $\{\mu_i(t)\}_{i=1}^r$ and $\{\nu_j(t)\}_{j=1}^s$ of $T(t)$ are continuous functions of $t$.

As noted in [10], the well–known continuity of $\lambda_1(t), \lambda_2(t), \ldots, \lambda_n(t)$ does not imply Theorem 4.5, since for a given $i$ the eigenvalue $\lambda_i(t)$ is even for some $t$ and odd for others.

The following result of Delsarte and Genin [3] implies that a repeated eigenvalue of an RST matrix $T$ is both even and odd.

Theorem 4.6. If $\lambda$ is an eigenvalue of an RST matrix $T$ with multiplicity $k > 1$ then the $\lambda$–eigenspace of $T$ has an orthonormal basis consisting of either $[k/2]$ symmetric and $[k/2]$ skew–symmetric $\lambda$–eigenvectors of $T$, or $[k/2]$ symmetric and $[k/2]$ skew–symmetric $\lambda$–eigenvectors of $T$.

5. Reformulation of Problem 1. The statement of Problem 1 does not reflect the current knowledge concerning the existence of its solution or the special spectral properties of RST matrices. We therefore reformulate Problem 1 as follows.

Problem 2. Given $n$ real numbers $\hat{\mu}_1 \leq \hat{\mu}_2 \leq \cdots \leq \hat{\mu}_r$ and $\hat{\nu}_1 \leq \hat{\nu}_2 \leq \cdots \leq \hat{\nu}_s$, find an $n$–vector $\hat{t}$ such that $\mu_i(\hat{t}) = \hat{\mu}_i, \ 1 \leq i \leq r$ and $\nu_j(\hat{t}) = \hat{\nu}_j, \ 1 \leq j \leq s$. 
We will call $\hat{\mu}_1, \hat{\mu}_2, \ldots, \hat{\mu}_r$ the *even target eigenvalues* and $\hat{\nu}_1, \hat{\nu}_2, \ldots, \hat{\nu}_s$ the *odd target eigenvalues*.

If $\tt$ is a solution of Problem 2 and $\tt'$ is obtained from $\tt$ by replacing $t_r$ by $(-1)^r t_r$, then $\tt'$ is also a solution of Problem 2 if $n$ is odd, or of Problem 2 with $\{\hat{\mu}_i\}$ and $\{\hat{\nu}_j\}$ interchanged if $n$ is even.

We say that the even and odd target eigenvalues $\{\hat{\mu}_i\}$ and $\{\hat{\nu}_j\}$ are *interlaced* if

$$\hat{\mu}_i \leq \hat{\nu}_i \leq \hat{\mu}_{i+1}, \quad 1 \leq i \leq m,$$

or if $n = 2m$ and either

$$\hat{\mu}_i \leq \hat{\nu}_i \leq \hat{\mu}_{i+1} \leq \hat{\nu}_m, \quad 1 \leq i \leq m - 1,$$

or

$$\hat{\nu}_i \leq \hat{\mu}_i \leq \hat{\nu}_{i+1} \leq \hat{\mu}_m, \quad 1 \leq i \leq m - 1.$$

A similar definition applies to the even and odd eigenvalues of an RST matrix $T(t)$.

By a nonconstructive argument based on topological degree (as proposed by Friedland [4]) Landau [7] has recently proved that Problem 2 always has a solution if $\{\hat{\mu}_i\}$ and $\{\hat{\nu}_j\}$ are interlaced. Delsarte and Genin [3] and Friedland [4] had established this earlier for $n \leq 4$.

In this paper we give a numerical procedure for solving Problem 2. We do not prove convergence; however, numerical experiments indicate that the procedure is globally convergent if $\{\hat{\mu}_i\}$ and $\{\hat{\nu}_j\}$ are interlaced, although in some instances it requires interaction on the part of the user, as explained in §9.

6. Newton’s method for Problem 2. Since the eigenvectors

$$p_1(t^{m-1}), p_2(t^{m-1}), \ldots, p_n(t^{m-1})$$

are associated with the $\lambda_1(t^{m-1}) < \lambda_2(t^{m-1}) < \cdots < \lambda_n(t^{m-1})$, it follows that (3) relates $\lambda_i(t^{m-1})$ to $\hat{\lambda}_i$ for $i = 1, \ldots, n$. This association is not appropriate for Problem 2, since in general $\lambda_i(t^{m})$ may be even for some values of $m$ and odd for others. Laurie mentioned an alternative association, which we paraphrase as follows, to be consistent with our terminology and notation: “the even and odd eigenvectors of $T(t^{m-1})$ are independently ordered, and interlaced afterwards, while still retaining the order of the target eigenvalues.” This is appropriate in the important special case where the even and odd target spectra are interlaced; however, Laurie’s stated motivation for proposing this procedure was his mistaken belief that Delsarte and Genin [3] had conjectured that the even and odd spectra of RST matrices are *always* interlaced. This is false (Laurie himself gave a counterexample in [8]), and Delsarte and Genin did not make this conjecture. Rather, by using Theorem 4.6 and a continuity argument, they showed that Problem 2 may fail to have a solution if $n \geq 4$ and $\{\hat{\mu}_i\}$ and $\{\hat{\nu}_j\}$ are not interlaced.

The results stated in the last two sections suggest that the iterative step indicated in (3) should be modified to associate $\mu_i(t^{m-1})$ with $\hat{\mu}_i$ for $1 \leq i \leq r$ and $\nu_j(t^{m-1})$ with $\hat{\nu}_j$ for $1 \leq j \leq s$. We will now describe this modification.

Let $p_1(t), \ldots, p_r(t), q_1(t), \ldots, q_s(t)$ be orthonormal symmetric and skew-symmetric eigenvectors of an RST matrix $T(t)$; thus,

$$T(t)p_i(t) = \mu_i(t)p_i(t), \quad 1 \leq i \leq r, \quad \text{and} \quad T(t)q_j(t) = \nu_j(t)q_j(t), \quad 1 \leq j \leq s.$$
(Theorem 4.6 implies that if $T(t)$ has no eigenvalues of multiplicity greater than two then $p_1(t), \ldots, p_r(t)$ and $q_1(t), \ldots, q_s(t)$ are uniquely defined up to sign.)

Henceforth $\Lambda$ will denote a vector

$$\Lambda = [\mu_1 \mu_2 \cdots \mu_r \nu_1 \nu_2 \cdots \nu_s]$$

in which

$$\mu_1 \leq \mu_2 \leq \cdots \leq \mu_r \quad \text{and} \quad \nu_1 \leq \nu_2 \leq \cdots \leq \nu_s.$$

Thus,

$$\Lambda(t) = [\mu_1(t) \mu_2(t) \cdots \mu_r(t) \nu_1(t) \nu_2(t) \cdots \nu_s(t)].$$

For a given $t$ and $\Lambda$ define

$$\sigma(t; \Lambda) = \|\Lambda(t) - \Lambda\| = \left( \sum_{i=1}^{r}(\mu_i(t) - \mu_i)^2 + \sum_{j=1}^{s}(\nu_j(t) - \nu_j)^2 \right)^{1/2}.$$

The following algorithm is an adaptation of Newton’s method for Problem 2; however, for flexibility of notation below, we denote the starting generator and target spectrum by $s^0$ and $\Lambda$ rather than $t^0$ and $\hat{\Lambda}$.

**Algorithm 6.1.** Let $s^0$ be a given $n$-vector, and let $\Lambda$ be as in (8) and (9). Define $s^0 = s$ and compute $s^m$ for $m \geq 1$ as the solution of the system

$$\begin{align*}
p_i(s^{m-1})^T T(s^m) p_i(s^{m-1}) &= \mu_i, \quad 1 \leq i \leq r, \\
q_j(s^{m-1})^T T(s^m) q_j(s^{m-1}) &= \nu_j, \quad 1 \leq j \leq s.
\end{align*}$$

If the even and odd target spectra are interlaced then the association between the eigenvectors of $T(s^{m-1})$ indicated in (11) is equivalent to Laurie’s alternate ordering procedure, discussed at the beginning of this section.

For computational purposes we write (11) more explicitly as

$$\sum_{k=1}^{n} a_{ik}(s^{m-1}) s^m_{k-1} = \mu_i, \quad 1 \leq i \leq r,$$

$$\sum_{k=1}^{n} b_{jk}(s^{m-1}) s^m_{k-1} = \nu_j, \quad 1 \leq j \leq s,$$

where

$$\begin{align*}
a_{ii}(s^{m-1}) &= 1, \quad 1 \leq i \leq r, \\
b_{ii}(s^{m-1}) &= 1, \quad 1 \leq j \leq s, \\
a_{ik}(s^{m-1}) &= 2 \sum_{l=1}^{n-k+1} p_{il}(s^{m-1}) p_{i,l+k-1}(s^{m-1}), \quad 2 \leq k \leq n, \quad 1 \leq i \leq r, \\
b_{jk}(s^{m-1}) &= 2 \sum_{l=1}^{n-k+1} q_{jl}(s^{m-1}) q_{j,l+k-1}(s^{m-1}), \quad 2 \leq k \leq n, \quad 1 \leq j \leq s.
\end{align*}$$
If $T(s^{m-1})$ has an eigenvalue of multiplicity greater than two then the eigenvectors in (11) are not uniquely defined; however, this never caused difficulty in literally thousands of experiments, even in cases where the target spectra contained elements of multiplicity greater than two.

We define Algorithm 6.1 to be successful if

$$\sigma(s^m; \Lambda) < \epsilon_0 \quad (14)$$

for some integer $m$, where $\epsilon_0$ defines the accuracy requirement. We must also define failure. We experimented with two kinds of definitions of failure, as follows.

(A) **Algorithm 6.1 fails if (14) does not occur for some $m \leq M$, where $M$ is a given integer.**

(B) **Algorithm 6.1 fails if the inequalities**

$$\sigma(s^m; \Lambda) \geq \sigma(s^{m-1}; \hat{\Lambda}) \geq \epsilon_0 \quad (15)$$

**occur a specified number $M_B$ of times. (Here $M_B$ is an integer; the subscript $B$ connotes "bad."**

Extensive numerical experimentation with the computational procedure described below has led us to conclude that criterion (B) with $M_B = 1$ is the most efficient criterion for failure. Thus, we have concluded empirically that if

$$\sigma(s^m; \hat{\Lambda}) < \sigma(s^{m-1}; \hat{\Lambda}), \quad m = 1, 2, \ldots, \quad (16)$$

then

$$\lim_{m \to \infty} \sigma(s^m; \Lambda) = 0, \quad \text{(17)}$$

and that even though (16) is not necessary for (17) it is, on the average, better to adopt a modified procedure (described below) if (15) occurs even once.

We cannot prove that (16) implies (17), but in thousands of trials we never encountered a case where (16) occurred while (17) did not; therefore, from a practical point of view, it seems safe to proceed on the assumption that (16) implies (17). The next definition is based on this assumption.

**Definition 6.2.** Suppose that $s^0$ is a given $n$-vector, $\Lambda$ is as in (8) and (9), and $\epsilon > 0$ where $\sigma(s^0; \Lambda) \geq \epsilon$. Let $\{s^m\}$ be as defined in Algorithm 6.1. If $M$ is the smallest integer such that

$$\sigma(s^m; \Lambda) < \sigma(s^{m-1}; \Lambda) \quad \text{for} \quad 1 \leq m \leq M \quad \text{and} \quad \sigma(s^M; \Lambda) < \epsilon,$$

then define $t(\Lambda; s^0; \epsilon) = s^M$; if there is no such integer $M$ then $t(\Lambda; s^0; \epsilon)$ is undefined.

Now suppose that we agree to accept a generator $t$ as a solution of Problem 2 if $\sigma(t; \hat{\Lambda}) < \epsilon_0$. Then we would accept

$$\hat{t} = t(\hat{\Lambda}; t^0; \epsilon_0)$$

as a solution if the vector on the right exists. Computational experiments with Algorithm 6.1 confirm what one would expect of Newton’s method: if $\{s^m\}$ converges then it converges quadratically. (This is true even if the target spectrum has repeated elements of multiplicity greater than two, which is consistent with results reported in [5].) Since Newton’s method is not globally convergent, $t(\hat{\Lambda}; t^0; \epsilon_0)$ may fail to exist.

The following lemma provides the basis for our procedure in this case.
Lemma 6.3. Suppose that the vector \( \hat{\Lambda} \) is the target spectrum in Problem 2, \( \rho \) is a number in \((0, 1)\), and \( t^0 \) is an arbitrary \( n \)-vector. For \( k \geq 1 \) suppose that \( t^k \) is an \( n \)-vector such that
\[
\Lambda(t^k) = (1 - \rho)\hat{\Lambda} + \rho\Lambda(t^{k-1}).
\] (18)
Then
\[
\sigma(t^k; \hat{\Lambda}) = \rho \sigma(t^{k-1}; \hat{\Lambda}).
\]

Proof. Since \( \hat{\Lambda} = (1 - \rho)\hat{\Lambda} + \rho\hat{\Lambda} \), (10) and (18) imply that
\[
\sigma(t^k; \hat{\Lambda}) = \|\Lambda(t^k) - \hat{\Lambda}\| = \rho\|\Lambda(t^{k-1}) - \hat{\Lambda}\| = \rho \sigma(t^{k-1}; \hat{\Lambda}).
\]

We propose the following algorithm for the case where Algorithm 6.1 fails with \( s^0 = t^0 \) and \( \Lambda = \hat{\Lambda} \).

Algorithm 6.4. Suppose that we agree to accept a generator \( \hat{t} \) as a solution to Problem 2 if \( \sigma(t; \hat{\Lambda}) < \epsilon_0 \), but Algorithm 6.1 fails with \( s = t^0 \) and \( \Lambda = \hat{\Lambda} \). Let \( \epsilon_1 \geq \epsilon_0 \) and \( \rho, \alpha \in (0, 1) \). (We will be more specific below about \( \epsilon_1, \alpha, \) and \( \rho \).) For \( k \geq 1 \), let
\[
t^k = t\left((1 - \rho)\hat{\Lambda} + \rho\Lambda(t^{k-1}); t^{k-1}; \alpha \sigma(t^{k-1}; \hat{\Lambda})\right).
\] (19)
Continue this procedure while \( \sigma(t^k; \hat{\Lambda}) \geq \epsilon_1 \). If \( K \) is the first integer such that
\[
\sigma(t^K; \hat{\Lambda}) < \epsilon_1,
\]
apply Algorithm 6.1 with \( s^0 = t^K \) and \( \Lambda = \hat{\Lambda} \), and accept
\[
\hat{t} = t(\hat{\Lambda}; t^K; \epsilon_0)
\]
as a solution of Problem 2.

Algorithm 6.4 has two phases. In the first we obtain \( t^k \) for \( 1 \leq k \leq K \) by solving Problem 2 with \( \hat{\Lambda} \) and \( t^0 \) replaced by \( (1 - \rho)\hat{\Lambda} + \rho\Lambda(t^{k-1}) \) and \( t^{k-1} \), subject to the accuracy requirement
\[
\sigma(t^k; \hat{\Lambda}) < \alpha \sigma(t^{k-1}; \hat{\Lambda}).
\] (21)
(This form for the accuracy requirement was motivated by experimental results.) Since
\[
\sigma(t^{k-1}; (1 - \rho)\hat{\Lambda} + \rho\Lambda(t^{k-1})) = (1 - \rho)\sigma(t^{k-1}; \hat{\Lambda}),
\]
it is reasonable to expect Algorithm 6.1 to yield a solution of this version of Problem 2 if \( (1 - \rho) \) is sufficiently small. We call this phase of Algorithm 6.4 the linear phase, since if the sequence \( \{t^k\} \) exists for some \( \rho \) then it converges linearly (with order \( \rho \)) to a solution of Problem 2. However, we continue the linear phase only until we obtain an iterate \( t^K \) that will serve as a successful starting generator for switching to Newton’s method for Problem 2 with target spectrum \( \hat{\Lambda} \). We call this second phase of Algorithm 6.4 the quadratic phase, since Newton’s method exhibits quadratic convergence.

Algorithm 6.4 fails if any of the applications of Algorithm 6.1 that it calls for fail. Our experiments indicate that there are generators \( t^0 \) with the following remarkable
property: given an arbitrary target spectrum \( \hat{\Lambda} \) with interlaced even and odd spectra, it is always possible to find \( \rho \) in \((0, 1)\) such that Algorithm 6.4 yields a solution to Problem 2. We cannot prove this assertion, and we hesitate to present it as a conjecture; however, we will discuss the computational evidence for it in \( \S 9 \).

We should point out that this is not the first attempt at formulating a global algorithm for the inverse eigenvalue problem for RST matrices. Laurie \[9\] proposed an algorithm that monitors the eigenvectors of the RST matrices produced in the iteration, rather than the matrices themselves. For reasons of length we will not go into the details of this algorithm, except to say that at each step the progress of the procedure is monitored and an appropriate choice is made between a locally quadratically convergent iterative method and a more cautious, locally linearly convergent method. The procedure does not exploit the special spectral properties of RST matrices, and is in fact proposed for a general class of inverse eigenvalue problems that contains Problem 1 as a special case. Numerical results with this algorithm are included for only one RST matrix of order 20, and compared with results obtained with Newton’s method. For that example both methods converged. Laurie states that Newton’s method was slightly faster.

\[ 7. \text{Choosing a starting generator.} \] Our earliest experiments convinced us that the version of Laurie’s algorithm discussed in \( \S 3 \) is virtually certain to fail if \( \{\mu_i(t^0)\} \) and \( \{\nu_j(t^0)\} \) are not interlaced. Similarly, except in contrived problems where \( \{\hat{\mu}_i\} \) and \( \{\hat{\nu}_j\} \) are sufficiently small perturbations of \( \{\mu_i(t^0)\} \) and \( \{\nu_j(t^0)\} \), Algorithms 6.1 and 6.4 are virtually certain to fail if either \( \{\hat{\mu}_i\} \) and \( \{\hat{\nu}_j\} \) are not interlaced or \( \{\mu_i(t^0)\} \) and \( \{\nu_j(t^0)\} \) are not interlaced. Fortunately, Landau’s theorem suggests that the most important case of Problem 2 is where \( \{\hat{\mu}_i\} \) and \( \{\hat{\nu}_j\} \) are interlaced. We consider only this case henceforth, and we require that \( \mathbf{T}(t^0) \) have \( n \) distinct eigenvalues and that \( \{\mu_i(t^0)\} \) and \( \{\nu_j(t^0)\} \) be interlaced. Results of the author \[10\] imply that \( \mathbf{T}(t^0) \) has these properties if

\[ t^0_r = \int_0^\pi f(\theta) \cos r\theta \, d\theta, \quad 1 \leq r \leq n - 1, \]  

where \( f \) is monotonic on \([0, \pi]\); if \( n = 2m \) then \( (6) \) applies if \( f \) is nondecreasing, while \( (7) \) applies if \( f \) is nonincreasing. Although monotonicity of \( f \) is not necessary for this conclusion, computational experiments indicate that the best starting generators are of the form \( (22) \) where \( f \) is continuous and strictly monotonic on \([0, \pi]\).

Laurie’s starting generator \((5)\) satisfies \( (22) \) with \( f(\theta) = \left(\frac{2}{\pi}\right) \cos \theta \). It is well known (see, for example, \[11\]) that the eigenvalues of the associated RST matrix are

\[ \lambda_k = -\frac{2}{\pi} \cos \left(\frac{k\pi}{n + 1}\right), \quad 1 \leq k \leq n, \]

with associated eigenvectors

\[ \mathbf{x}_k = [x_{1k}, x_{2k}, \ldots, x_{nk}]^T, \quad 1 \leq k \leq n, \]

where

\[ x_{mk} = (-1)^m \sin \left(\frac{km\pi}{n + 1}\right), \quad 1 \leq m \leq n. \]  

Although it is not stated in \[8\] that the tridiagonal RST matrix generated by \((5)\) has interlaced even and odd spectra (Laurie said he chose \((5)\) because of the simple
formula (23) for the eigenvectors), this undoubtedly explains Laurie’s success with (5).

However, it seems reasonable that a starting generator \( t^0 \) such that \( T(t^0) \) has essentially equally spaced eigenvalues would be better on the average, and experimental results confirm this. Szegő’s theory on the asymptotic distribution of the eigenvalues of Hermitian Toeplitz matrices [6] implies that generators obtained from (22) with \( f(\theta) = \theta \) have this property for large \( n \). In fact, for practical purposes, this is true for all \( n \) of interest.

Consistent with our normalization (1), (2), we used starting generators of the form

\[
(24) \quad t^0 = [0 \ t_1^0 \cdots t_{n-1}^0]
\]

satisfying (22) with monotonic \( f \), where

\[
(25) \quad 2\sum_{r=1}^{n-1} (n-r)(t_r^0)^2 = 1,
\]

so that \( T(t^0) \) has trace zero and Frobenius norm one.

In this paper we report only on results obtained with with starting generators satisfying (22) with \( f(\theta) = J_n \cos \theta \) and \( f(\theta) = -K_n \theta \), where \( J_n \) and \( K_n \) are both positive and chosen so that the corresponding generator satisfies (25). (We choose the minus sign in the second function merely so that both functions are decreasing on \((0, \pi)\) and the relative orderings of the interlaced even and odd spectra of the RST matrices that they generate are the same; that is, the largest eigenvalue is even for any \( n \).) Thus, the two generators are of the form (24), with

\[
(26) \quad t_r = \begin{cases} 
0 & \text{if } r = 1, \\
\frac{1}{2(n-1)} & \text{if } r \neq 1,
\end{cases}
\]

which is Laurie’s generator (normalized), and

\[
(27) \quad t_r = \begin{cases} 
\frac{1}{M_n r^2} & \text{if } r \text{ is odd}, \\
0 & \text{if } r \text{ is even},
\end{cases} \quad \text{with } M_n = \left( \sum_{r=1}^{n-1} (1 + (-1)^r) \left( \frac{n-r}{r^2} \right) \right)^{1/2}.
\]

We also experimented with several other starting generators associated as in (22) with monotonic functions. Our results indicated that (27) is probably the best “general purpose” starting generator. For reasons of length we do not include results of experiments with the starting generators other than (26) and (27).

8. Computational strategy. Our program is written in MATLAB. To obtain the eigenvalues and eigenvectors of RST matrices we apply standard MATLAB procedures to the associated matrices \( A \) and \( B \) defined in Theorems 4.1–4.4. By exploiting the symmetry and skew–symmetry of the eigenvectors the number of operations required to compute the the coefficients \( a_{ik}(s^{n-1}) \) and \( b_{jk}(s^{n-1}) \) by means of (12) and (13) is approximately halved.

The primary inputs to the program are the target spectrum \( \hat{\Lambda} \) and the starting generator \( t^0 \). (It is to be understood in the following that these are normalized as in (1) and (2), since this is the first step in the computation.) The other inputs are the parameters \( \rho, \alpha, \epsilon_0 \), and \( \epsilon_1 \) defined in Algorithm 6.4, and a number \( \Delta \rho \in (0, 1) \).
The default mode for the computation is as follows.

**Step 1.** If \( \rho = 0 \) execute Algorithm 6.1 with \( s^0 = t^0 \) and \( \Lambda = \hat{\Lambda} \). If \( t(\hat{\Lambda}; t^0; \epsilon_0) \) (Definition 6.2) exists then accept it as a solution of Problem 2. If \( t(\hat{\Lambda}; t^0; \epsilon_0) \) does not exist then set \( \rho = \Delta \rho \) and proceed with Step 2.

**Step 2.** If \( 0 < \rho < 1 \) then execute Algorithm 6.4. If the vector \( t(\hat{\Lambda}; t^K; \epsilon_0) \) defined in Algorithm 6.4 exists, then accept it as a solution of Problem 2. If \( t(\hat{\Lambda}; t^K; \epsilon_0) \) does not exist then replace \( \rho \) by \( \rho + \Delta \rho \). If this new value of \( \rho \) is \( \geq 1 \) then cease computing and admit defeat; if it is \( < 1 \) then repeat Step 2.

In §9 we will also discuss a variation of this procedure that is useful for solving Problem 2 with “pathological” target spectra, as defined there.

In each pass through Step 2 we use the original starting generator \( t^0 \). This may seem wasteful, since the failed computation will in general have produced generators that are closer to a solution of Problem 2 than \( t^0 \); however, computational experiments show that it is not good to use a generator obtained in a failed attempt with Step 1 as a starting generator for Step 2, or to use a generator obtained in a failed pass through Step 2 as a starting generator for the next pass (with a larger value of \( \rho \)).

**9. Experimental results.** In all of the experiments reported here we worked with interlaced even and odd target spectra normalized as in (1) and (2), and took

\[
\epsilon_0 = 10^{-14} \quad \text{and} \quad \Delta \rho = .1.
\]

All computations were performed on personal computers equipped with Intel 486 chips. Because of memory limitations we took \( n \leq 200 \) in all experiments.

In the first set of experiments that we will report on the target spectra were generated as follows.

1. Start with \( x = [x_1 \ x_2 \ \cdots \ x_n]^T \), in which the components are independent normally distributed random numbers with mean 0 and variance 1, computed with MATLAB’s “randn” function.

2. Rearrange the components of \( x \) to obtain \( y = [y_1 \ y_2 \ \cdots \ y_n]^T \), in which

\[
y_i \leq y_{i+1}, \ 1 \leq i \leq n - 1.
\]

3. Compute

\[
\bar{y} = \frac{1}{n}(y_1 + y_2 + \cdots + y_n) \quad \text{and} \quad S = \left( \sum_{i=1}^{n} (y_i - \bar{y})^2 \right)^{1/2}.
\]

4. Let the target spectrum be \( \hat{\Lambda} = [\hat{\lambda}_1 \ \hat{\lambda}_2 \ \cdots \ \hat{\lambda}_n] \) with \( \hat{\lambda}_i = (y_i - \bar{y})/S \) (so that \( \hat{\Lambda} \) satisfies (1) and (2)) and allocate \( \hat{\lambda}_1, \hat{\lambda}_2, \ldots, \hat{\lambda}_n \) alternately between the even and odd target spectra, so that \( \hat{\lambda}_n \) is even.

We considered target spectra of this kind for \( n = 25, 50, 100, 150, \) and 200, and solved Problem 2 for 100 target spectra of each order. The results are shown in Tables 1–4, all of which deal with the same target spectra. In these computations we took \( \epsilon_1 = 10^{-4} \) in (20); that is, we stayed in the linear phase of Algorithm 6.4 until we obtained a starting generator \( t^K \) such that \( \sigma(t^K; \hat{\lambda}) < 10^{-4} \). We took \( \alpha \) in (19) to be either .01 or .1. For these choices of \( \alpha \), obtaining \( t^K \) from \( t^{K-1} \) by means of (19) was usually accomplished with one (sometimes two, rarely more) passes through Algorithm 6.1, once the appropriate value of \( \rho \) was found by means of the procedure outlined in Step 2.
Table 1 shows the results obtained with $\alpha = .01$ and Laurie’s (normalized) starting generator (26). The first column of the table shows the possible choices of $\rho$. Since we start with $\rho = 0$ and have taken $\Delta \rho = .1$, there are ten possibilities: with $\rho = 0$ in Step 1 or with $\rho = .1, .2, \ldots, 9$ in Step 2. Note that there are two columns in the table corresponding to each value of $n$. The first column shows the number of solutions obtained with the corresponding values of $\rho$, while the second column shows the average total number of iterations required to obtain them. (The number of iterations required to obtain a solution is defined to be the total number of times it is required to solve the system (11), starting with Step 1.) Thus, with $n = 50$, 64 solutions were obtained with $\rho = 0$, with an average of 7.05 iterations per solution; 28 solutions were obtained with $\rho = .1$, with an average of 11.93 iterations per solution; 6 solutions were obtained with $\rho = .2$, with an average of 16.33 iterations per solution; and 2 solutions were obtained with $\rho = .3$, with an average of 18.00 iterations per solution. The number $\bar{\tau}$ in the bottom row of the table is the overall average number of iterations required per solution; thus, $\bar{\tau} = 9.19$ for $n = 50$. Tables 2–4 are to be interpreted similarly.

Table 2 shows the results obtained with $\alpha = .01$ and the starting generator (27); thus, the only difference between the results summarized in Tables 1 and 2 is the choice of starting generator. Comparing Tables 1 and 2 shows that the starting generator (27) is on the average superior to Laurie’s generator (26).

Table 3 presents results obtained under the same conditions as those in Table 2, except that $\alpha$ has been increased from .01 to .1; thus the accuracy requirement (21) in the linearly convergent phase of Algorithm 6.4 has been relaxed. Comparing Tables 2
Table 3
100 Randomly Generated Targets of Order $n$; $\alpha = .1$; Starting Generator (27)

<table>
<thead>
<tr>
<th>$\rho$</th>
<th>$n =$ 25</th>
<th>$n =$ 50</th>
<th>$n =$ 100</th>
<th>$n =$ 150</th>
<th>$n =$ 200</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>86</td>
<td>68</td>
<td>56</td>
<td>45</td>
<td>26</td>
</tr>
<tr>
<td></td>
<td>5.93</td>
<td>6.65</td>
<td>7.25</td>
<td>7.82</td>
<td>8.15</td>
</tr>
<tr>
<td>0.1</td>
<td>13</td>
<td>31</td>
<td>41</td>
<td>46</td>
<td>63</td>
</tr>
<tr>
<td></td>
<td>9.23</td>
<td>10.16</td>
<td>10.51</td>
<td>11.24</td>
<td>11.48</td>
</tr>
<tr>
<td>0.2</td>
<td>1</td>
<td>14.00</td>
<td>3</td>
<td>8</td>
<td>8</td>
</tr>
<tr>
<td></td>
<td>12.00</td>
<td>15.33</td>
<td>15.88</td>
<td>14.75</td>
<td></td>
</tr>
<tr>
<td>0.3</td>
<td>0</td>
<td>0.00</td>
<td>0</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td></td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>19.00</td>
<td>18.00</td>
</tr>
<tr>
<td>$\bar{\tau}$</td>
<td>6.43</td>
<td>7.79</td>
<td>8.83</td>
<td>10.15</td>
<td>11.07</td>
</tr>
</tbody>
</table>

Table 4
100 Randomly Generated Targets of Order $n$; $\alpha = .1$; Initial $\rho = .1$; Starting Generator (27)

<table>
<thead>
<tr>
<th>$\rho$</th>
<th>$n =$ 25</th>
<th>$n =$ 50</th>
<th>$n =$ 100</th>
<th>$n =$ 150</th>
<th>$n =$ 200</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>98</td>
<td>97</td>
<td>97</td>
<td>89</td>
<td>88</td>
</tr>
<tr>
<td></td>
<td>6.91</td>
<td>7.38</td>
<td>7.81</td>
<td>8.15</td>
<td>8.41</td>
</tr>
<tr>
<td>0.2</td>
<td>2</td>
<td>3</td>
<td>3</td>
<td>10</td>
<td>9</td>
</tr>
<tr>
<td></td>
<td>10.00</td>
<td>10.33</td>
<td>11.67</td>
<td>12.90</td>
<td>12.11</td>
</tr>
<tr>
<td>0.3</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td></td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>17.00</td>
<td>16.00</td>
</tr>
<tr>
<td>$\bar{\tau}$</td>
<td>6.97</td>
<td>7.47</td>
<td>7.93</td>
<td>8.71</td>
<td>8.97</td>
</tr>
</tbody>
</table>

and Table 3 shows that this yielded a slight improvement.

It can be seen from Table 3 that Step 1 fails to produce a solution in a significant number of cases, and this number increases with $n$. Table 4 presents results obtained under the same conditions as those of Table 3, except that Step 1 is omitted; that is $\rho = .1$ initially. Comparing Tables 3 and 4 shows that this resulted in improvement for $n = 50, 100, 150$, and 200, but not for $n = 25$, for which there were many (86) successes with $\rho = 0$.

Table 3 shows that our procedure produced solutions of Problem 2 with errors less than $10^{-14}$ for all 500 of the randomly generated normalized spectra, starting with $t_0$ as in (27) and taking $\alpha = .1$ and $\epsilon_1 = 10^{-4}$. The solutions were obtained in Step 1 ($\rho = 0$) in 281 cases, while the other 219 were obtained in Step 2 with $\rho \leq .4$.

In these computations $\epsilon_1 = 10^{-4}$ is much larger than $\epsilon_0 = 10^{-14}$; that is, we switch from the linear to the quadratic phase of Algorithm 6.4 while still quite far from a solution of Problem 2. Our results show that this procedure is effective with randomly generated target spectra. However, it must to be modified in some cases where there are repeated target eigenvalues or – worse – clusters of target eigenvalues very close to each other. In many such cases – particularly those in which there are multiple exactly equal (i.e., to full machine precision) target eigenvalues, Step 1 still produces a solution. However, it is often necessary to invoke Step 2. In this case it may be necessary to handle the transition from the linear to the quadratic phase of Algorithm 6.4 more carefully, since the quadratic phase may fail if $\epsilon_1$ is larger than the the difference between “almost equal” target eigenvalues. If this happens with a given value of $\rho$, we restart the linear phase of Algorithm 6.4 with the same value of $\rho$ and a smaller value of $\epsilon_1$, taking the starting generator to be the vector $t^0$ that satisfied (20) with the previous choice of $\epsilon_1$. There are then two possibilities:

(a) The linear phase of Algorithm 6.4 is successful with the new choice of $\epsilon_1$, so we enter the quadratic phase. If this is successful, then we are finished; if not, we repeat the procedure just described with a still smaller $\epsilon_1$.

(b) The linear phase of Algorithm 6.4 fails with the new choice of $\epsilon_1$. In this case we replace $\rho$ by $\rho + \Delta \rho$, retain the new choice of $\epsilon_1$, and restart Algorithm 6.4 with the original starting generator $t^0$. 

Table 5
Results for prolate spheroidal target spectra with starting generator (26)

<table>
<thead>
<tr>
<th>(n)</th>
<th>25</th>
<th>50</th>
<th>75</th>
<th>100</th>
<th>150</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\rho)</td>
<td>.1</td>
<td>.3</td>
<td>.3</td>
<td>.3</td>
<td>.4</td>
</tr>
<tr>
<td>(\epsilon_1)</td>
<td>(10^{-6})</td>
<td>(10^{-11})</td>
<td>(10^{-9})</td>
<td>(10^{-12})</td>
<td>(10^{-12})</td>
</tr>
<tr>
<td>(c_{\rho})</td>
<td>12</td>
<td>25</td>
<td>23</td>
<td>27</td>
<td>35</td>
</tr>
</tbody>
</table>

Table 6
Results for prolate spheroidal target spectra with starting generator (27)

<table>
<thead>
<tr>
<th>(n)</th>
<th>25</th>
<th>50</th>
<th>75</th>
<th>100</th>
<th>150</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\rho)</td>
<td>.1</td>
<td>.3</td>
<td>.3</td>
<td>.4</td>
<td>.4</td>
</tr>
<tr>
<td>(\epsilon_1)</td>
<td>(10^{-9})</td>
<td>(10^{-12})</td>
<td>(10^{-12})</td>
<td>(10^{-12})</td>
<td>(10^{-12})</td>
</tr>
<tr>
<td>(c_{\rho})</td>
<td>14</td>
<td>26</td>
<td>27</td>
<td>35</td>
<td>35</td>
</tr>
</tbody>
</table>

In every experiment with pathological target spectra in which we used (27) as a starting generator, we were able to find combinations of \(\rho\) and \(\epsilon_1\) such that Algorithm 6.4 produced a solution to Problem 2. There were some extreme cases in which we were forced to take \(\epsilon_1\) so close to \(\epsilon_0 = 10^{-14}\) that Algorithm 6.4 never entered its quadratic phase; that is, the sequence \(\{t^k\}\) defined by (19) converged linearly (with order of convergence \(\rho\)) to \(t\).

Among the numerous experiments that we performed with pathological target spectra were some in which the target spectra were obtained by normalizing the spectra of the modified prolate spheroidal matrices \(P_n = (p_{i-j})_{i,j=1}^{n}\), where

\[
p_r = \begin{cases} 
0, & r = 0, \\
\sin r \pi / 2 / r \pi, & 1 \leq r \leq n - 1,
\end{cases}
\]

for which the eigenvalue problem is notoriously difficult because the eigenvalues of \(P\) are clustered equally about \(\lambda = -1/2\) and \(\lambda = 1/2\), and the tightness of the clustering increases very rapidly with \(n\). By applying our algorithm interactively as just described, we were able to solve Problem 2 with \(n = 25, 50, 75, 100,\) and \(150\) for these target spectra, with \(\epsilon_0 = 10^{-14}\). We took \(\alpha = .1\) in all cases. Tables 5 and 6 summarize the results obtained with using the starting generators (26) and (27), respectively. The second column of Table 5, for example, indicates that with \(n = 25\) we obtained a solution with \(c_{\rho} = 12\) iterations after determining that the appropriate choices for \(\rho\) and \(\epsilon_1\) were \(.1\) and \(10^{-6}\), respectively. The other columns are to be interpreted similarly. It is interesting to note that Laurie’s starting generator outperformed (27) for these target spectra.

10. Summary. We believe that the main contributions of this paper are as follows:

1. It presents a formulation of Newton’s method for the solution of the inverse eigenvalue problem for RST matrices which takes account of the special spectral properties of RST matrices, including the separation of their spectra into even and odd parts, Landau’s existence theorem [7] for the existence of a solution with interlaced even and odd spectra, the related possible nonexistence result of Delsarte and Genin [3], and the computational efficiency implicit in the results of Cantoni and Butler [2] (Theorems 4.1–4.4).
2. It emphasizes that the starting generator should generate an RST matrix with interlaced even and odd spectra. In particular, it proposes a new starting generator (27) which seems to be superior to the previously suggested starting generator (26) for most target spectra.

3. It presents a criterion for abandoning Newton’s method with a given starting generator and a locally linearly convergent procedure for determining a new starting generator if Newton’s method shows signs of failure.

4. It reports the results of extensive numerical experimentation.

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