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NUMERICAL SOLUTION OF THE EIGENVALUE PROBLEM FOR SYMMETRIC RATIONALLY GENERATED TOEPLITZ MATRICES*

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Abstract. A numerical method is proposed for finding all eigenvalues of symmetric Toeplitz matrices $T_n = (t_{j-i})_{i,j=1}^n$, where the $\{t_j\}$ are the coefficients in a Laurent expansion of a rational function. Matrices of this kind occur, for example, as covariance matrices of ARMA processes. The technique rests on a representation of the characteristic polynomial as det $(\lambda I_n - T_n) = W_n G_{0n} G_{1n}$ in which $G_{0n}(\lambda) = 0$ for the eigenvalues of T_n associated with symmetric eigenvectors, $G_{1n}(\lambda) = 0$ for those associated with skew-symmetric eigenvectors, both functions are free of extreme variations, and both can be computed with cost independent of n. It is proposed that root finding techniques be used to compute the zeros of G_{0n} and G_{1n}. Numerical experiments indicate that the method may be useful.

Key words. Toeplitz, rationally generated, eigenvalue, eigenvector

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1. Introduction.

Let

$$A(z) = a_0 + a_1 z + \cdots + a_q z^q$$

and

$$C(z) = \sum_{j=-p}^{p} c_j z^j,$$

where $a_0, \cdots, a_q$ and $c_{-p}, \cdots, c_0, \cdots, c_p$ are real, $c_j = c_{-j} (1 \leqq j \leqq p)$, $a_q c_p \neq 0$, and $A(z)$ has no zeros in $|z| \leqq 1$. Then the rational function

$$T(z) = \frac{C(z)}{A(z)A(1/z)}$$

has a convergent Laurent expansion

$$T(z) = \sum_{j=-\infty}^{\infty} t_j z^j \tag{1}$$

(with $t_j = t_{-j}$) in an open annulus containing $|z| = 1$.

Here we propose a numerical method for determining the eigenvalues of the symmetric Toeplitz matrices

$$T_n = (t_{j-i})_{i,j=1}^n .$$

Matrices of this kind occur, for example, as covariance matrices of wide-sense stationary autoregressive-moving average time series. (In this setting, $C(z) = B(z)B(1/z)$, with $B(z) = b_0 + b_1 z + \cdots + b_p z^p$.) This is a preliminary report in that further numerical experimentation is required to ascertain whether the method works well for large values of

$$m = \max (p, q); \tag{2}$$

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however, computations already performed with $m = 1, 2$, and 3 indicate that the method can be used very successfully to obtain *all* eigenvalues of T_n at a cost per eigenvalue which depends essentially only on m and is independent of n.

The asymptotic distribution of the eigenvalues of sequences of Toeplitz matrices T_n associated with a convergent Laurent series has been studied extensively. (See, e.g., [8], [13], [19], [20]; there are many other references.) Recently there have been several papers on the spectral structure of symmetric Toeplitz matrices (e.g., [2]–[4], [6], [9]–[11], [15], [16]); however, little has been published on methods for computing the eigenvalues of Toeplitz matrices by methods specifically designed to exploit their simple structure (e.g., [2], [5], [7], [12], [14]). To the author's knowledge, nothing of this kind has been published for rationally generated symmetric Toeplitz matrices, except for the papers of Bini and Capovani [2] and Katai and Rahmy [14], both of which deal only with the case where $A(z) = 1$, so that T_n is banded if $n > q$.

Although it is generally agreed that applying root finding techniques to locate the zeros of its characteristic polynomial is not a good way to find the eigenvalues of a high-order matrix, we believe that this is a viable method for the matrices that we are considering. In order to demonstrate this, we need a theorem proved in [18].

Let $\theta_{-q}, \cdots, \theta_q$ be defined by

$$A(z)A(1/z) = \sum_{j=-q}^{q} \theta_j z^j \tag{3}$$

and define

$$c_j = 0 \quad \text{if } |j| > p, \qquad \theta_j = 0 \quad \text{if } |j| > q.$$

Let $\tau_0, \tau_1, \cdots$ be the Chebyshev polynomials, i.e.,

$$\tau_n(\cos t) = \cos nt. \tag{4}$$

Finally, let

$$p_n(\lambda) = \det [\lambda I_n - T_n]$$

be the characteristic polynomial of T_n, and define

$$C_{rn}(\gamma) = \sum_{j=0}^{q} a_j \cos (n + 2r - 2j - 1)\gamma \tag{5}$$

and

$$S_{rn}(\gamma) = \sum_{j=0}^{q} a_j \sin (n + 2r - 2j - 1)\gamma. \tag{6}$$

Our approach is based on the following theorem, which is proved in [18].

THEOREM 1. *Let λ be such that $c_m - \lambda\theta_m \neq 0$ and the polynomial*

$$P(w; \lambda) = c_0 - \lambda\theta_0 + 2 \sum_{j=1}^{m} (c_j - \lambda\theta_j)\tau_j(w) \tag{7}$$

has m distinct zeros $w_1, \cdots, w_m$ such that

$$w_s \neq 1 \quad or -1, \qquad 1 \leqq s \leqq m, \tag{8}$$

and let

$$\gamma_s = \frac{1}{2} \cos^{-1} w_s, \qquad 0 \leqq \operatorname{Re} (\gamma_s) \leqq \frac{\pi}{2}. \tag{9}$$

Then

(10) $$p_n(\lambda) = K_n(c_m - \lambda\theta_m)^n F_{0n}(\lambda)F_{1n}(\lambda),$$

where K_n *is a constant,*

(11) $$F_{0n}(\lambda) = \frac{\det [C_{rn}(\gamma_s)]_{r,s=1}^m}{\det [\cos (2r-1)\gamma_s]_{r,s=1}^m},$$

and

(12) $$F_{1n}(\lambda) = \frac{\det [S_{rn}(\gamma_s)]_{r,s=1}^m}{\det [\sin (2r-1)\gamma_s]_{r,s=1}^m}.$$

Moreover, if $F_{ln}(\lambda) = 0$ ($l = 0$ *or* 1), *then* T_n *has a* λ*-eigenvector*

$$U = [u_1, \cdots, u_n]^t$$

such that

(13) $$u_{n-i+1} = (-1)^l u_i, \qquad 1 \leqq i \leqq n.$$

We will follow Cantoni and Butler [3] and say that U is *symmetric* if (13) holds with $l = 0$, or *skew-symmetric* if (13) holds with $l = 1$. In [3] it is shown that if T_n is an $n \times n$ real symmetric Toeplitz matrix, then R^n has an orthonormal basis consisting of $n - [n/2]$ symmetric and $[n/2]$ skew-symmetric eigenvectors of T_n. (Here $[x]$ is the integer part of x.) For convenience we will say that the *even spectrum* of T_n consists of eigenvalues with associated symmetric eigenvectors, while the *odd spectrum* consists of eigenvalues with associated skew-symmetric eigenvectors.

Finding the zeros of $P(z; \lambda)$ for a given λ is a nontrivial but tractable (particularly for $1 \leqq m \leqq 4$) problem. Therefore, (10), (11), and (12) *in principle* provide a means for computing $p_n(\lambda)$ for a given λ, with computational cost independent of n, which enters into them only as a parameter. Nevertheless, it is clearly impractical to apply root finding techniques directly to $p_n(\lambda)$ if n is large, simply because a polynomial of high degree can assume tremendous values between its zeros. Fortunately, Theorem 1 provides a way to overcome this difficulty. We will use Theorem 1 to obtain simpler functions which can be evaluated for a given λ with computational cost independent of n, have the same zeros as $F_{0n}(\lambda)$ and $F_{1n}(\lambda)$, and do not vary wildly between their zeros. Root finding techniques can be successfully applied to these functions.

If $m = 1$ in (2), our approach reduces the eigenvalue problem to routine computations and solves it completely (in the numerical sense). We will therefore consider this case separately in § 2. However, some general comments are in order first.

Let

(14) $$f(t) = \frac{C(e^{it})}{A(e^{it})A(e^{-it})}, \qquad -\pi \leqq t \leqq \pi.$$

Then f is real-valued, and $f(t) = f(-t)$; moreover, (3), (4), (7), and (14) imply the identity

(15) $$P(\cos t; f(t)) = 0, \qquad -\pi \leqq t \leqq \pi.$$

It is easily seen that the $\{t_j\}$ in (1) are the Fourier coefficients of f; therefore, if

(16) $$a = \min_{0 \leq t \leq \pi} f(t), \qquad b = \max_{0 \leq t \leq \pi} f(t),$$

then the eigenvalues of T_n are all in $[a, b]$ for every n (see [8, p. 64]).

For convenience, we will say that the values of λ which do not satisfy the conditions of Theorem 1 are *exceptional points* of $P(\ ;\lambda)$. All other values of λ will be called *ordinary points*. There are at most finitely many exceptional points, and each is of one of the following types: (i) The point $\lambda = c_m/\theta_m$, if $\theta_m \neq 0$. (ii) A value of λ for which the resultant $R(\lambda)$ of the polynomials $P(w;\lambda)$ and $P_w(w;\lambda)$ vanishes; since $R(\lambda)$ is a polynomial in λ, there are only finitely many of these. (iii) The numbers $f(0)$ and $f(\pi)$, since, from (15), $P(1, f(0)) = 0$, $P(-1, f(\pi)) = 0$, which violates (8).

2. The case $m = 1$. If $m = 1$, then $T(z)$ can be written as

$$T(z) = \frac{c_0 + c_1(z + 1/z)}{(1 - \rho z)(1 - \rho/z)}, \tag{17}$$

with $-1 < \rho < 1$. If $\rho = 0$, then T_n is a tridiagonal Toeplitz matrix, and the eigenvalue problem can be solved explicitly (e.g., see [17]). Therefore, we assume that $\rho \neq 0$. We also assume that

$$\rho c_0 + (1 + \rho^2)c_1 = \alpha \neq 0, \tag{18}$$

which guarantees that $T(z)$ does not reduce to a constant, since

$$f'(t) = \frac{-2\alpha \sin t}{(1 - 2\rho \cos t + \rho^2)^2}. \tag{19}$$

Subject to these assumptions, it is straightforward to obtain the expansion (1), with

$$t_j = \frac{c_1 \rho^{|j-1|} + c_0 \rho^{|j|} + c_1 \rho^{|j+1|}}{1 - \rho^2}.$$

Kac, Murdock, and Szegö [13] have considered the special case where

$$c_0 = 1 - \rho^2, \qquad c_1 = 0. \tag{20}$$

The general case can be reduced to this by applying long division to (17), but this would not shorten our presentation. Our results are more detailed than theirs, as we will indicate below.

With T as in (17), (7) becomes

$$P(w;\lambda) = c_0 - \lambda(1 + \rho^2) + 2(c_1 + \lambda\rho)w.$$

Our assumption (18) and its consequence (19) imply that $f(0)$ and $f(\pi)$ are the endpoints of the interval $[a, b]$ defined by (16), and that $c_1 + \lambda\rho \neq 0$, $P(1;\lambda) \neq 0$, and $P(-1;\lambda) \neq 0$ if $a < \lambda < b$. Therefore, Theorem 1 implies that

$$p_n(\lambda) = \frac{K_n(c_1 + \lambda\rho)^n C_n(\gamma) S_n(\gamma)}{\cos\gamma \sin\gamma}, \qquad a < \lambda < b, \tag{21}$$

where K_n is a constant,

$$\gamma = \frac{1}{2}\cos^{-1}\left[\frac{\lambda(1 + \rho^2) - c_0}{2(c_1 + \lambda\rho)}\right], \qquad 0 < \gamma < \frac{\pi}{2},$$

$$C_n(\gamma) = \cos(n+1)\gamma - \rho\cos(n-1)\gamma, \tag{22}$$

and

$$S_n(\gamma) = \sin(n+1)\gamma - \rho\sin(n-1)\gamma. \tag{23}$$

The formula given in [8] and [13] for the characteristic polynomial of the Kac–Murdock–Szegö matrix

$$T_n = (\rho^{|j-i|})_{i,j=1}^n,$$

obtained by choosing c_0 and c_1 as in (20), is

$$p_n(\lambda) = \frac{(-\lambda\rho)^n H_n(\gamma)}{(1-\rho^2)\sin 2\gamma}, \tag{24}$$

with

$$H_n(\gamma) = \sin(2n+2)\gamma - 2\rho \sin 2n\gamma + \rho^2 \sin(2n-2)\gamma \tag{25}$$

and

$$\gamma = \frac{1}{2}\cos^{-1}\left[\frac{\lambda(1+\rho^2)-(1-\rho^2)}{2\lambda\rho}\right]. \tag{26}$$

It is observed in [8] that if $H_n(\gamma) = 0$ for some γ in $(0, \pi/2)$, then solving (26) for λ produces an eigenvalue of T_n. It is also shown in [8] that the zeros $\gamma_1, \cdots, \gamma_n$ of H_n satisfy the inequalities

$$0 < \gamma_1 < \frac{\pi}{2n+2} < \gamma_2 < \frac{2\pi}{2n+2} \cdots < \gamma_n < \frac{n\pi}{2n+2}$$

if $0 < \rho < 1$. (The case where $-1 < \rho < 0$ was not considered in [8].)

Numerical computations were not considered in [8], but it is clear that, given such precise information on their locations, $\gamma_1, \cdots, \gamma_n$ can easily be obtained by applying the method of regula falsi to H_n. Therefore, this classical example already illustrates the feasibility of finding the eigenvalues of these matrices by the direct application of root finding techniques, not to $p_n(\lambda)$ itself, but to the simple function $H_n(\gamma)$.

Further insight into the eigenvalue problem for this case can be gained by the factorization

$$H_n(\gamma) = 2C_n(\gamma)S_n(\gamma)$$

(cf. (22), (23), (25)), which shows that (21) and (24) are equivalent if (20) holds. Theorem 1 implies that if $C_n(\gamma) = 0$ for some γ in $(0, \pi/2)$ then the quantity

$$\lambda = \frac{c_0 + 2c_1 \cos 2\gamma}{1 - 2\rho\cos 2\gamma + \rho^2} \tag{27}$$

is in the even spectrum of T_n. Also, if $S_n(\gamma) = 0$, then λ in (27) is in the odd spectrum of T_n.

By rewriting (22) and (23) as

$$C_n(\gamma) = (1 - \rho\cos 2\gamma)\cos(n+1)\gamma - \rho\sin 2\gamma \cdot \sin(n+1)\gamma$$

and

$$S_n(\gamma) = (1 - \rho\cos 2\gamma)\sin(n+1)\gamma + \rho\sin 2\gamma \cdot \cos(n+1)\gamma,$$

and then noticing the signs of C_n and S_n at the points

$$x_j = \frac{j\pi}{n+1}, \qquad 0 \leqq j \leqq n - [n/2],$$

and

$$y_j = \frac{(j+\frac{1}{2})\pi}{n+1}, \qquad 0 \leqq j \leqq [n/2],$$

it is straightforward to verify that (i) if $0 < \rho < 1$, then C_n has a zero in (x_{j-1}, y_{j-1}) for each $j = 1, \cdots, n - [n/2]$ and S_n has a zero in (y_{j-1}, x_j) for each $j = 1, \cdots, [n/2]$; (ii) if $-1 < \rho < 0$, then C_n has a zero in (y_{j-1}, x_j) for each $j = 1, \cdots, n - [n/2]$, and S_n has a zero in (x_j, y_j) for each $j = 1, \cdots, [n/2]$.

In either case these zeros are easy to locate by the method of regula falsi. We have written very short BASIC programs to find the zeros and compute the eigenvalues of the Kac–Murdock–Szegö matrices. To illustrate the ease with which they solve the problem, we cite two examples connected with the matrix

$$T_{1000} = (2^{-|j-i|})_{i,j=1}^{n},$$

with computations performed on an IBM PC AT.

(a) With single precision arithmetic (seven significant decimal figures) and requiring the regula falsi iterations to continue until the successive estimates of the zeros of $C_n(\gamma)$ (or $S_n(\gamma)$) agreed in the first six figures, it took 185 seconds to compute the 1000 eigenvalues of T_{1000}.

(b) With double precision arithmetic (16 significant decimal digits) and requiring the regula falsi iterations to continue until the successive estimates of the zeros agreed to 15 places, it took eight minutes to compute the same eigenvalues (of course, to considerably better accuracy than that obtained in (a)).

Since the right side of (27) is a monotonic function of γ in $(0, \pi/2)$ (its derivative, except for a constant, is given by (19) with $t = 2\gamma$), our results imply that the odd and even spectra of T_n are interlaced. This has been previously observed by Delsarte and Genin [6].

In the proof of Theorem 1 we gave a general formula ([18, eq. (38)]) for the eigenvectors of rationally generated symmetric matrices. For the special case considered in this section, this formula implies that if $C_n(\gamma) = 0$ and λ from (27) is the corresponding eigenvalue, then a corresponding (symmetric) eigenvector is given by $U = [u_1, \cdots, u_n]^t$, with

$$u_i = \cos(n-2i+1)\gamma, \qquad 1 \leqq i \leqq n.$$

If $S_n(\gamma) = 0$, then

$$u_i = \sin(n-2i+1)\gamma, \qquad 1 \leqq i \leqq n,$$

which defines a skew-symmetric eigenvector.

3. The general case ($m \geqq 2$). Now suppose that $m \geqq 2$ and λ is an ordinary point. Then (10), (11), and (12) enable us *in principle* to evaluate $p_n(\lambda)$ with computational cost independent of n, but they suffer from the defect that even though $p_n(\lambda)$ is clearly real if λ is real, (11) and (12) involve complex numbers unless $w_1, \cdots, w_m$ are all in the interval $(-1, 1)$, which is not so in general. Moreover, the tremendous range of values that $p_n(\lambda)$ can assume make it impractical to apply root finding methods directly to $p_n(\lambda)$, or perhaps even to compute it at all.

Fortunately, these problems can be overcome. We will now show that on any subinterval $[a_1, b_1]$ of $[a, b]$ (cf. (16)) containing only ordinary points of $P(\ ;\lambda)$, we can write

$$p_n(\lambda) = W_n(\lambda)G_{0n}(\lambda)G_{1n}(\lambda) \tag{28}$$

where W_n "absorbs" the large variations of $p_n(\lambda)$, but has no zeros on $[a_1, b_1]$ and is therefore of no interest, while G_{0n} and G_{1n} are reasonably computable functions, involving only real quantities, to which root finding methods such as the method of regula falsi or one of its variants can be applied. The zeros of G_{0n} and G_{1n} are, respectively, the elements of the even and odd spectra of T_n which lie in $[a_1, b_1]$.

We need the following lemma, which is established by invoking elementary properties of algebraic functions (see, e.g., [1]) and recalling that P in (7) has real coefficients.

LEMMA 1. *The equation $P(w; \lambda) = 0$ defines m continuous (in fact, analytic) functions $w_i = w_i(\lambda)$ $(1 \leqq i \leqq m)$ on any interval $[a_1, b_1]$ consisting entirely of ordinary points of $P(\ ; \lambda)$. Moreover, for each $i = 1, \cdots, m$; (i) $w_i(\lambda)$ is real for some λ in $[a_1, b_1]$ if and only if it is real for all such λ; (ii) if w_i is real-valued, then the functions $w_i - 1$ and $w_i + 1$ have no zeros on $[a_1, b_1]$.*

This lemma enables us to factor p_n as in (28), where

$$G_{0n}(\lambda) = \det\,[\check{C}_{rn}(\gamma_s)]_{r,s=1}^{m}$$

and

$$G_{1n}(\lambda) = \det\,[\check{S}_{rn}(\gamma_s)]_{r,s=1}^{m}.$$

For each s the definition of $\check{C}_{rn}(\gamma_s)$ and $\check{S}_{rn}(\gamma_s)$ depends upon whether (i) $-1 < w_s < 1$, (ii) $w_s > 1$, (iii) $w_s < -1$, or (iv) w_s is complex. Lemma 1 implies that exactly one of these conditions holds for all λ in $[a_1, b_1]$.

Case (i). $-1 < w_s < 1$. Here $C_{rn}(\gamma_s)$ and $S_{rn}(\gamma_s)$ are simply linear combinations of (real) sines and cosines, so we let $\check{C}_{rn}(\gamma_s) = C_{rn}(\gamma_s)$, and $\check{S}_{rn}(\gamma_s) = S_{rn}(\gamma_s)$.

In the remaining cases (9) implies that $\gamma_s = \alpha_s + i\beta_s$, where

$$\cos 2\alpha_s \cosh 2\beta_s = u_s, \quad \sin 2\alpha_s \sinh 2\beta_s = -v_s, \quad 0 \leqq \alpha_s \leqq \frac{\pi}{2} \tag{29}$$

with $w_s = u_s + iv_s$.

Case (ii). $w_s > 1$. Then $w_s = u_s$ and $v_s = 0$ in (29); hence,

$$\alpha_s = 0 \quad \text{and} \quad \beta_s = \tfrac{1}{2}\cosh^{-1} w_s;$$

hence, from (5) and (6),

$$C_{rn}(\gamma_s) = \sum_{j=0}^{q} a_j \cosh\,(n + 2r - 2j - 1)\beta_s \tag{30}$$

and

$$S_{rn}(\gamma_s) = i \sum_{j=0}^{q} a_j \sinh\,(n + 2r - 2j - 1)\beta_s. \tag{31}$$

The imaginary unit in the last equation cancels with one which occurs in column s of the denominator in (12). To eliminate large variations, we factor $e^{n\beta_s}/2$ out of the sums in (30) and (31), and define

$$\check{C}_{rn}(\gamma_s) = \sum_{j=0}^{q} a_j[e^{(2r-2j-1)\beta_s} + e^{-(2n+2r-2j-1)\beta_s}],$$

$$\check{S}_{rn}(\gamma_s) = \sum_{j=0}^{q} a_j[e^{(2r-2j-1)\beta_s} - e^{-(2n+2r-2j-1)\beta_s}].$$

The exponential factor is simply included in $W_n(\lambda)$. Note that $\check{C}_{rn}(\gamma_s)$ and $\check{S}_{rn}(\gamma_s)$ are bounded for all n. This will also be true in the following cases.

Case (iii). $w_s < -1$. Now

$$\gamma_s = \frac{\pi}{2} + i\beta_s,$$

with

$$\beta_s = \tfrac{1}{2} \cosh^{-1}(-w_s);$$

hence (5) and (6) imply that

$$\pm \sum_{j=0}^{q} (-1)^j a_j \cosh (n+2r-2j-1)\beta_s = \begin{cases} C_{rn}(\gamma_s) & \text{if } n \text{ is odd,} \\ S_{rn}(\gamma_s) & \text{if } n \text{ is even} \end{cases}$$

and

$$\pm i \sum_{j=0}^{q} (-1)^j a_j \sinh (n+2r-2j-1)\beta_s = \begin{cases} S_{rn}(\gamma_s) & \text{if } n \text{ is odd,} \\ C_{rn}(\gamma_s) & \text{if } n \text{ is even.} \end{cases}$$

Therefore, we remove the exponential factor and irrelevant constants as before, and define

$$\sum_{j=0}^{q} (-1)^j a_j [e^{(2r-2j-1)\beta_s} + e^{-(2n+2r-2j-1)\beta_s}] = \begin{cases} \check{C}_{rn}(\gamma_s) & \text{if } n \text{ is odd,} \\ \check{S}_{rn}(\gamma_s) & \text{if } n \text{ is even} \end{cases}$$

and

$$\sum_{j=0}^{q} (-1)^j a_j [e^{(2r-2j-1)\beta_s} - e^{-(2n+2r-2j-1)\beta_s}] = \begin{cases} \check{S}_{rn}(\gamma_s) & \text{if } n \text{ is odd,} \\ \check{C}_{rn}(\gamma_s) & \text{if } n \text{ is even.} \end{cases}$$

Case (iv). $w_s = u_s + iv_s$, $v_s \neq 0$. For real λ the coefficients in (7) are real; hence, we may assume without loss of generality that

(32) $$w_{s+1} = u_s - iv_s.$$

If

(33) $$\tau = \cosh^2 2\beta_s,$$

then (29) implies that

$$\frac{u_s^2}{\tau} + \frac{v_s^2}{\tau - 1} = 1,$$

or

$$(\tau - 1)u_s^2 + \tau v_s^2 = \tau(\tau - 1).$$

Solving this quadratic equation and noting that $\tau > 1$ yields

$$\tau = \tfrac{1}{2}(1 + u_s^2 + v_s^2 + \sqrt{(1 + u_s^2 + v_s^2)^2 - 4u_s^2}).$$

Now (29) and (33) imply that

$$\alpha_s = \tfrac{1}{2} \cos^{-1} (u_s/\sqrt{\tau})$$

and

(34) $$\beta_s = \tfrac{1}{2}\,\mathrm{sgn}\,(-v_s)\cosh^{-1}\sqrt{\tau}.$$

It now follows from (5) and (6) that

(35) $$\begin{aligned} C_{rn}(\gamma_s) = &\sum_{j=0}^{q} a_j \cos(n+2r-2j-1)\alpha_s \cosh(n+2r-2j-1)\beta_s \\ &- i\sum_{j=0}^{q} a_j \sin(n+2r-2j-1)\alpha_s \sinh(n+2r-2j-1)\beta_s \end{aligned}$$

and

(36) $$\begin{aligned} S_{rn}(\gamma_s) = &\sum_{j=0}^{q} a_j \sin(n+2r-2j-1)\alpha_s \cosh(n+2r-2j-1)\beta_s \\ &+ i\sum_{j=0}^{q} a_j \cos(n+2r-2j-1)\alpha_s \sinh(n+2r-2j-1)\beta_s \end{aligned}$$

are the elements in the sth columns of the determinants in the numerators of (11) and (12), respectively. But now (32) and (34) imply that $\gamma_{s+1} = \alpha_s - i\beta_s$, so the elements in the $(s+1)$st columns of these matrices are the conjugates of (35) and (36), i.e.,

$$C_{rn}(\gamma_{s+1}) = \overline{C_{rn}(\gamma_s)}, \qquad S_{rn}(\gamma_{s+1}) = \overline{S_{rn}(\gamma_s)}.$$

This and elementary properties of determinants imply that replacing $C_{rn}(\gamma_s)$ and $C_{rn}(\gamma_{s+1})$ in columns s and $s+1$ of $\det [C_{rn}(\gamma_s)]_{r,s=1}^{n}$ by Re $(C_{rn}(\gamma_s))$ and Im $(C_{rn}(\gamma_s))$ simply multiplies this determinant by a purely imaginary constant (which is cancelled by the same constant produced by similar manipulations on the determinant in the denominator of (11)). Following this by factoring out the exponential $e^{n|\beta_s|}$ and other constants leads us to define the elements in column s of $G_{0n}(\lambda)$ by

$$\tilde{C}_{rn}(\gamma_s) = \sum_{j=0}^{q} a_j[e^{(2r-2j-1)|\beta_s|} + e^{-(2n+2r-2j-1)|\beta_s|}]\cos(n+2r-2j-1)\alpha_s$$

and the elements in column $s+1$ by

$$\tilde{C}_{rn}(\gamma_{s+1}) = \sum_{j=0}^{q} a_j[e^{(2r-2j-1)|\beta_s|} - e^{-(2n+2r-2j-1)|\beta_s|}]\sin(n+2r-2j-1)\alpha_s.$$

Similar operations on the real and imaginary parts of (36) lead to the definitions

$$\tilde{S}_{rn}(\gamma_s) = \sum_{j=0}^{q} a_j[e^{(2r-2j-1)|\beta_s|} + e^{-(2n+2r-2j-1)|\beta_s|}]\sin(n+2r-2j-1)\alpha_s$$

and

$$\tilde{S}_{rn}(\gamma_{s+1}) = \sum_{j=0}^{q} a_j[e^{(2r-2j-1)|\beta_s|} - e^{-(2n+2r-2j-1)|\beta_s|}]\cos(n+2r-2j-1)\alpha_s$$

as the entries in columns s and $s+1$ of $G_{1n}(\lambda)$.

4. A proposed procedure for finding all eigenvalues of T_n. Here we assume that $m \geqq 2$, since § 2 reduces the case where $m = 1$ to routine computations. We propose a procedure for computing all the eigenvalues of T_n. As mentioned earlier, it is known that the spectrum of T_n is contained in the interval $[a, b]$. For simplicity we will assume here that the eigenvalues $\lambda_{1n}, \cdots, \lambda_{nn}$ are distinct, that no exceptional point of $P(\ ;\lambda)$ is an eigenvalue, and that

$$a<\lambda_{1n}<\lambda_{2n}<\cdots<\lambda_{nn}<b.$$

We consider two situations: (I) the eigenvalues of T_{n-1} are already known and satisfy the inequalities

$$a<\lambda_{1,n-1}<\lambda_{2,n-1}<\cdots<\lambda_{n-1,n-1}<b;$$

and (II) the eigenvalues of T_{n-1} are not known.

The first requirement of the procedure is to subdivide $[a, b]$ into closed subintervals $I_1, \cdots, I_k$ with disjoint interiors such that none of the I_j's contains more than one eigenvalue from each of the even and odd spectra. This is very easily done in situation (I); we simply let $k = n$ and

$$I_j=\begin{cases}[a,\lambda_{1,n-1}] & \text{if } j=1,\\ [\lambda_{j-1,n-1},\lambda_{j,n-1}] & \text{if } 2\leqq j\leqq n-1,\\ [\lambda_{n-1,n-1},b] & \text{if } j=n.\end{cases}$$

Since T_{n-1} is a principal submatrix of T_n, standard separation theorems imply that each of the intervals $I_1, \cdots, I_n$ contains exactly one eigenvalue of T_n.

Obtaining the desired subdivision of $[a, b]$ in situation (II) requires some guesswork, but the guessing is of the educated variety, thanks to the celebrated theorem of Szegö which says that for large n the eigenvalues of T_n are distributed in $[a, b]$ like the ordinates

$$f\left(\frac{j\pi}{n+1}\right),\qquad 1\leqq j\leqq n. \tag{37}$$

(For a more precise statement of this result see [8] or [20].) Motivated by this, we have used the following procedure to subdivide $[a, b]$: compute the ordinates (37), list them in memory, and construct a new list $g_1, \cdots, g_n$ consisting of these numbers arranged in nondecreasing order. (Since f' cannot have more than $2m-2$ zeros on $(0, \pi)$, this can be accomplished efficiently, even for large n.) Then define $g_0 = a$ and $g_{n+1} = b$. In the numerical experiments that we have performed with $m = 2$ and 3 the intervals $I_j = [g_{j-1}, g_j]$, $1 \leqq j \leqq n+1$ usually satisfy our requirements even for small values of n, like $n = 5$ or $n = 10$. (We would expect that the probability of success with this procedure would increase with n, due to the asymptotic nature of Szegö's theorem. It should also be noted that we do not require that no interval contain more than one eigenvalue; because of our factorization of the characteristic polynomial, an interval may contain two eigenvalues, provided that one belongs to the even spectrum of T_n and the other to the odd.) In some cases we missed a few of the eigenvalues. We then used the "brute force" approach of simply dividing all the intervals into k parts (usually with k arbitrarily chosen to be 5). Obviously, this strategy can be improved.

Now we describe the computations performed for each interval in the subdivision. Let $I = [c, d]$, where it is assumed that I does not contain more than one element from each of the odd and even spectra of T_n and that c and d are not eigenvalues of T_n. Suppose first that I contains only ordinary points of $P(\ ;\lambda)$, and let G_{0n} and G_{1n} be the functions defined on I in § 4. If

$$G_{ln}(c)G_{ln}(d)<0 \tag{38}$$

for $l = 0$ ($l = 1$), then I contains exactly one element from the even (odd) spectrum of T_n, which can be computed by applying the method of regula falsi to G_{qn}. If (38) does not hold for either $l = 0$ or $l = 1$, then I contains no eigenvalues of T_n.

Now suppose that I contains one or more exceptional points. In this case the definition of G_{qn} will in general change on I. Now we simply subdivide I into subintervals whose interiors contain no exceptional points, pick slightly smaller closed subintervals of these which contain no exceptional points (hoping that no eigenvalue actually lies in the small part of I that is excluded in this process), and apply the above procedure to these intervals. This strategy has worked well in all cases considered.

5. Typical numerical experiments for $m = 2$ and $m = 3$. The computations performed so far have been done with BASIC/D (double precision) programs on an IBM PC AT. No attempt has as yet been made to use more sophisticated programming techniques or numerical methods (such as improvements on the method of regula falsi to find the zeros of G_{0n} and G_{1n}); the objective of these computations was simply to ascertain whether there was any hope that this method would work. The results are quite encouraging. The following are typical examples.

Example 1. We took

$$A(z) = \left(1 - \frac{z}{10}\right)\left(1 - \frac{z}{5}\right)$$

and

$$C(z) = 1.5 - 3.5(z + z^{-1}) + (z^2 + z^{-2}).$$

Regula falsi iterations were continued until successive iterates agreed in the first 15 significant decimal digits. The running times to obtain all eigenvalues of T_n were 0:54 (minutes and seconds) with $n = 10$, 3:44 with $n = 50$, 6:40 with $n = 100$, and slightly over 98 minutes with $n = 1000$. (The last required time seems to be longer than we would expect, given the first three. The author does not know the reason for this.)

Example 2. We took

$$A(z) = 1 - .4z - .47z^2 + .21z^3$$

and

$$C(z) = 1 + 2(z + z^{-1}) - (z^2 + z^{-2}) + (z^3 + z^{-3}).$$

The regula falsi iterations were continued until successive iterates agreed to 12 significant decimal digits. The running times required to compute all eigenvalues were 3:58, 12:56, and 22:10 for $n = 10$, 50, and 100, respectively.

We have obtained partial checks on our results. For example, all of our test computations yielded eigenvalue distributions consistent with what we would expect from Szegö's distribution theorem, and in all cases the eigenvalues of T_n separated those of T_{n+1}.

6. Conclusions and further research. Numerical results obtained so far indicate that this method is an efficient way to compute the eigenvalues of high-order symmetric rationally generated Toeplitz matrices with $m = 1$, 2, or 3 in (2). Since the scaling of G_{0n} and G_{1n} makes these functions bounded for all n, there seems to be no reason why the procedure cannot be applied to very high order matrices, particularly since it does not require that the elements of T_n be stored, or even computed. Moreover, it is obvious that much greater computing speeds can be obtained by using more sophisticated programming methods and/or equipment. We believe that the major problems which need to be overcome in order to apply this method efficiently for larger values of m in (2) are as follows.

(i) Efficient methods must be developed to find the zeros of $P(\ ;\lambda)$ for a given λ. For $m = 1, 2, 3$ we have simply used standard formulas for the zeros of a polynomial in terms of its coefficients. This method is also a possibility for $m = 4$, but root-finding methods are obviously required for $m \geqq 5$. Of course, there are standard methods available for this problem; moreover, if λ_k and λ_{k+1} are successive iterates obtained in a regula falsi procedure, then the zeros $w_1(\lambda_k), \cdots, w_m(\lambda_k)$ should be reasonably good first approximations to $w_1(\lambda_{k+1}), \cdots, w_m(\lambda_{k+1})$.

(ii) An improved version of the method of regula falsi should be devised. This would include the more or less standard procedure of combining it with bisection, which accelerates convergence in certain situations (i.e., where one endpoint would otherwise "stay in the game" for an excessive number of iterations). It is not clear how further improvements could be attained; for example, iterative methods (such as Newton's) which require the computation of derivatives would not be useful, since we have no computable formulas for the derivatives of G_{0n} and G_{1n} in terms of the zeros of $P(\ ;\lambda)$. Moreover, it seems desirable to insist that the iterative method be one that is guaranteed to converge.

(iii) Accurate computation of the $m \times m$ determinants defining G_{0n} and G_{1n} may be difficult for larger values of m. This does not appear to be a problem for $m = 2$ and $m = 3$. In fact, for $m = 3$ we treated this problem in two ways: (a) a simple cofactor expansion and (b) reduction to triangular form with full pivoting. Although the second method would presumably be more accurate for larger m, there was no difference between the results obtained by the two methods for $m = 3$.

Another area of investigation would be to compute the eigenvectors associated with the eigenvalues obtained by this procedure and check the residuals

$$\alpha = \frac{\|T_n X - \lambda X\|}{\|X\|}.$$

This would be a formidable computation if carried out by brute force; however, the formula given in [18] for the eigenvectors of T_n should greatly simplify this calculation.

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