A NOTE ON COMPUTING EIGENVALUES OF BANDED HERMITIAN TOEPLITZ MATRICES

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Abstract. It is pointed out that the author's $O(n^2)$ algorithm for computing individual eigenvalues of an arbitrary $n \times n$ Hermitian Toeplitz matrix T_n reduces to an $O(rn)$ algorithm if T_n is banded with bandwidth r.

Suggested running head: BANDED TOEPLITZ EIGENVALUE PROBLEM

AMS (MOS) Mathematics Subject Classifications: 65F15, 15A18, 15A57

Key words and phrases: Toeplitz, Hermitian, banded, eigenvalue, eigenvector.

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A Note on Computing Eigenvalues of
Banded Hermitian Toeplitz Matrices

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In a recent paper Arbenz [2] (see also [1]) presented a method for computing the eigenvalues of a Toeplitz matrix

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

where

$$t_\nu = t_{-\nu} \quad \text{and} \quad t_\nu = 0 \text{ if } |\nu| > r;$$

thus, T_n is symmetric. If $n > r$ (which we assume henceforth), then T_n is also banded. Following Arbenz, we will say that T_n *has bandwidth* r.

Since [2] is so recent and easily accessible, there is no need to go into the details of Arbenz's algorithm here; rather, we focus on the important point that it yields the eigenvalues of T_n with a computational cost of $O(r(n+r^2))$ flops per eigenvalue. Another approach to this problem is discussed in [3] and [6].

It seems worthwhile to point out that the quite different algorithm given by the author in [9] for finding individual eigenvalues of a full Hermitian Toeplitz matrix with $O(n^2)$ flops per eigenvalue requires only $O(rn)$ flops per eigenvalue in the banded case. Here we will give the briefest description of the algorithm that suffices to make this point. For complete details, see [9]. For related results, see [10].

Theorems 1 and 2 of [9] imply the following theorem, which is the basis for the algorithm.

THEOREM 1. *Let* T_n *be a Hermitian Toeplitz matrix, let* T_m $(1 \le m \le n)$ *be its* $m \times m$ *principal submatrix, and define*

$$q_m(\lambda) = \frac{p_m(\lambda)}{p_{m-1}(\lambda)}, \ 1 \le m \le n,$$

where

$$p_0(\lambda) = 1 \quad and \quad p_m(\lambda) = \det[T_m - \lambda I_m], \ 1 \le m \le n.$$

If λ is not an eigenvalue of any of the principal submatrices $T_1, \ldots, T_{n-1}$, then $q_1(\lambda), \ldots, q_n(\lambda)$ can be computed recursively as follows. Let

$$q_1(\lambda) = t_0 - \lambda, \qquad x_{11}(\lambda) = t_1/(t_0 - \lambda).$$

Then, for $2 \le m \le n - 1$,

$$q_m(\lambda) = [1 - |x_{m-1,m-1}(\lambda)|^2] q_{m-1}(\lambda),$$

$$x_{mm}(\lambda) = (q_m(\lambda))^{-1} [t_m - \sum_{j=1}^{m-1} t_j x_{m-j,m-1}(\lambda)], \tag{2}$$

and

$$x_{jm}(\lambda) = x_{j,m-1}(\lambda) - x_{mm}(\lambda)\bar{x}_{m-j,m-1}(\lambda), \ 1 \le j \le m - 1. \tag{3}$$

Finally,

$$q_n(\lambda) = [1 - |x_{n-1,n-1}(\lambda)|^2] q_{n-1}(\lambda).$$

Moreover, if λ is an eigenvalue of T_n, then

$$Y_n(\lambda) = \begin{bmatrix} -1 \\ X_{n-1}(\lambda) \end{bmatrix}$$

is an associated eigenvector, where

$$X_{n-1}(\lambda) = \begin{bmatrix} x_{1,n-1}(\lambda) \\ x_{2,n-1}(\lambda) \\ \vdots \\ x_{n-1,n-1}(\lambda) \end{bmatrix}.$$

Let the eigenvalues of T_n be

$$\lambda_1 \le \lambda_2 \le \ldots \le \lambda_n,$$

and suppose that we wish to compute λ_k for a given k in $\{1, 2, \ldots, n\}$. We assume that λ_k is not an eigenvalue of any of the submatrices $T_1, \ldots, T_{n-1}$. From Sturm's theorem, the number of negative values in $\{q_1(\lambda), q_2(\lambda), \ldots, q_m(\lambda)\}$ equals the number of eigenvalues of $T_m - \lambda I_m$ less than λ. Therefore, if we can guess values a and b such that $\lambda_k \in (a, b)$, then Theorem 1 and bisection can be used to find a subinterval (α, β) of (a, b) which contains λ_k but no other eigenvalue of T_n nor any eigenvalue of T_{n-1}. Since q_n is continuous on (α, β), we can then use a more elaborate iterative rootfinder to compute λ_k as a zero of q_n. In [9] and [10] we chose the Pegasus modification [5, 7] of the rule of false position, which has order of convergence approximately 1.642. If $\{\mu_j\}$ is the sequence of iterates produced by the Pegasus computation, starting with $\mu_0 = \alpha$ and $\mu_1 = \beta$, then we terminate this phase of the computation at the first integer r such that

$$|\mu_r - \mu_{r-1}| < .5(1 + \mu_r)10^{-K}, \tag{4}$$

where K is a positive integer dictated by machine precision and accuracy requirements.

For a full Hermitian Toeplitz matrix T_n the computations in Theorem 1 require approximately n^2 flops for each λ. Therefore, the computation of each eigenvalue requires $0(n^2)$ flops, where the "constant" buried in the "0" depends on the number of iterations required for the given eigenvalue. Although this number depends upon the eigenvalue itself and on the starting values (a and b), computational experience (see [9]) shows that for a given choice of K in (4), its average value over all eigenvalues of a matrix of order n is essentially independent of n. Thus, we can say that the cost of the procedure is roughly $M(K)n^2$ flops per eigenvalue. (For the computations reported in [9], $M(10) \approx 11$.) However, the point of the present note is that if T_n is banded, then the computations in Theorem 1 require only $O(rn)$ flops, so the algorithm in [9] yields eigenvalues of T_n at a cost of $O(rn)$ flops per eigenvalue. The reason for this is the following theorem, which is easily obtained from Theorem 1. We omit the proof.

THEOREM 2. *In addition to the assumptions of Theorem 1, let T_n have bandwidth $r < n$. Then $q_1(\lambda), \ldots, q_n(\lambda)$ can be computed recursively as in Theorem 1, except that if $m > r$ then (2) and (3) can be replaced by*

$$x_{mm}(\lambda) = -(q_m(\lambda))^{-1} \sum_{j=1}^{r} t_j x_{m-j,m-1}(\lambda), \tag{5}$$

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and

$$x_{jm}(\lambda) = x_{j,m-1}(\lambda) - x_{mm}(\lambda)\bar{x}_{m-j,m-1}(\lambda), \ 1 \leq j \leq r \quad and \quad m-r \leq j \leq m-1 \tag{6}$$

if $m \geq r+1$.

It is significant that the summation in (5) involves only r products rather than $m-1$ as in (2), and we compute only $2r$ (fewer if $r < m < 2r$) components of $X_{n-1}(\lambda)$ in (6), as compared to m in (3). Therefore, Theorem 2 implies that for large n the algorithm of [9] requires approximately $(3r+1)n$ flops to compute $q_0(\lambda), q_1(\lambda), \ldots, q_n(\lambda)$ for a given λ if T_n has bandwidth r. Since numerical experiments indicate no significant differences between convergence properties of the algorithm for banded and full matrices, this means that the average cost of computing a single eigenvalue of a banded Hermitian Toeplitz matrix is $M(K)(3r+1)n$ flops, where $M(10) \approx 11$ if $K = 10$ in (4).

Having obtained λ_k by computations based on Theorems 1 and 2, we have as a byproduct the first $r+1$ components

$$y_{1n}(\lambda_k) = -1, y_{2n}(\lambda_k) = x_{1,n-1}(\lambda_k), \ldots, y_{r+1,n}(\lambda_k) = x_{r,n-1}(\lambda_k)$$

and the last r components

$$y_{n-r+1,n}(\lambda_k) = x_{n-r,n-1}(\lambda_k), \ldots, y_{nn} = x_{n-1,n-1}(\lambda_k)$$

of the associated eigenvector $Y_n(\lambda_k)$. However, the last r components are not independent, since if λ_k is a simple eigenvalue of T_n, then either

$$y_{n-i+1,n}(\lambda_k) = y_{in}(\lambda_k) \text{ or } y_{n-i+1,n}(\lambda_k) = -y_{in}(\lambda_k), \ 1 \leq i \leq n,$$

[4]. In any case, even if λ_k has multiplicity greater than one, the first r components of $Y_n(\lambda_k)$ determine the rest. To see this, we recall from [8] that the components of $Y_n(\lambda_k)$ satisfy the difference equation

$$\sum_{j=-r}^{r} t_j y_{i+j,n}(\lambda_k) = \lambda_k y_{in}(\lambda_k), \ 1 \leq i \leq n, \tag{7}$$

subject to the boundary conditions

$$y_{in}(\lambda_k) = 0, \ -r+1 \leq i \leq 0, \tag{8}$$

and

$$y_{in}(\lambda_k) = 0, \ n+1 \le i \le n+r.$$

Therefore, if

$$y_{1n}(\lambda_k), \ldots, y_{rn}(\lambda_k) \tag{9}$$

are known, then the remaining components of $Y_n(\lambda_k)$ can in principle be obtained by treating (8) as initial conditions and computing recursively from (7):

$$y_{i+r,n}(\lambda_k) = -\frac{1}{t_r} \sum_{j=-r}^{r-1} (t_j - \delta_{0j}\lambda_k)y_{i+j,n}(\lambda_k), \ i \ge 1. \tag{10}$$

Since the zeros of the characteristic polynomial

$$P(z) = \sum_{j=-r}^{r} t_j z^j - \lambda_k$$

of (7) occur in reciprocal pairs, the recursion (10) is unstable and therefore computationally useless; nevertheless, it proves our assertion that the components (9) completely determine $Y_n(\lambda_k)$.

From this it seems reasonable to make the (admittedly vague) conjecture that any meaningful question depending upon the eigenvector $Y_n(\lambda_k)$ can in principle be resolved from a knowledge of the components in (9), without actually computing the remaining ones. However, if the remaining components are required, then it is useful to recall from [9] that $X_{n-1}(\lambda_k)$ is the solution of the banded Toeplitz system

$$(T_{n-1} - \lambda_k I_{n-1})X = \begin{bmatrix} t_1 \\ t_2 \\ \vdots \\ t_r \\ 0 \\ \vdots \\ 0 \end{bmatrix}.$$

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This is a tractable problem, since there are several well known fast algorithms for solving banded Toeplitz systems.

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