



A symmetry exploiting Lanczos method for symmetric Toeplitz matrices

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Dedicated to Richard S. Varga on the occasion of his 70th birthday

Several methods for computing the smallest eigenvalues of a symmetric and positive definite Toeplitz matrix T have been studied in the literature. Most of them share the disadvantage that they do not reflect symmetry properties of the corresponding eigenvector. In this note we present a Lanczos method which approximates simultaneously the odd and the even spectrum of T at the same cost as the classical Lanczos approach.

Keywords: Toeplitz matrix, eigenvalue problem, Lanczos method, symmetry

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1. Introduction

Several approaches have been reported in the literature for computing the smallest eigenvalue of a real symmetric, positive definite Toeplitz matrix. This problem is of considerable interest in signal processing. Given the covariance sequence of the observed data, Pisarenko [21] suggested a method which determines the sinusoidal frequencies from the eigenvector of the covariance matrix associated with its minimum eigenvalue.

Cybenko and Van Loan [4] presented an algorithm which is a combination of bisection and Newton's method for the secular equation. Replacing Newton's method by a root finding method based on rational Hermitian interpolation of the secular equation Mackens and the present author in [16,17] improved this approach. Hu and Kung [11] considered a safeguarded inverse iteration with Rayleigh quotient shifts, and Huckle [13,14] studied the spectral transformation method. Trench [23] and Noor and Morgera [20] generalized the method of Cybenko and Van Loan to the computation of the complete spectrum. A disadvantage of all of these approaches is that none of them exploits symmetry properties of the eigenvectors.

Let $J_n = (\delta_{i,n+1-i})_{i,j=1,\dots,n}$ denote the (n, n) flipmatrix with ones in its secondary diagonal and zeros elsewhere. A vector $x \in \mathbb{R}^n$ is called symmetric if $x = J_n x$, and it is called skew-symmetric (or antisymmetric) if $x = -J_n x$. It is well known (cf. [2,3]) even

for the larger class of symmetric and centrosymmetric matrices that every eigenspace of a matrix C_n in this class (i.e., $c_{n+1-i, n+1-j} = c_{ij}$ for every $i, j = 1, \dots, n$) has a basis of vectors which are either symmetric or skew-symmetric, and that there exists a basis of \mathbb{R}^n consisting of $\lceil n/2 \rceil$ symmetric and $\lfloor n/2 \rfloor$ skew-symmetric eigenvectors of C_n . We call an eigenvalue λ of C_n even (odd) if there is a corresponding eigenvector which is symmetric (skew-symmetric).

For symmetric Toeplitz matrices Delsarte and Genin [5] proved that the symmetric and skew-symmetric eigenvalues are the roots of separate secular equations which have better numerical properties than the joint one. Taking advantage of a more convenient form of the even and odd secular equations (which were independently derived by Melman [18,19]) we improved the methods of [16,17] for computing the smallest eigenvalue of a symmetric Toeplitz matrix in [26,27]. The even equation was already used by Huang [12] to determine the smallest even eigenvalue of a Toeplitz matrix.

Andrew [2], Cantoni and Butler [3] and Trench [24] (the latter for symmetric Toeplitz matrices only) exploited symmetry properties of symmetric and centrosymmetric matrices to reduce the eigenvalue problem to two eigenproblems of half the dimension. For a symmetric Toeplitz matrix $T_n \in \mathbb{R}^n$, $T_n = (t_{|i-j|})$, their approach is as follows:

If $n = 2m$ is even then T_n may be written as

$$T_n = \begin{pmatrix} T_m & \tilde{H}_m \\ \tilde{H}_m^T & T_m \end{pmatrix}, \quad \tilde{H}_m = \begin{pmatrix} t_m & t_{m+1} & \dots & t_{n-1} \\ t_{m-1} & t_m & \dots & t_{n-2} \\ \vdots & \vdots & \ddots & \vdots \\ t_1 & t_2 & \dots & t_m \end{pmatrix}.$$

If $x = J_n x$ is a symmetric eigenvector of T_n then it holds that $x = [\tilde{x}; J_m \tilde{x}]$, $\tilde{x} := x(1 : m) \in \mathbb{R}^m$, and

$$T_n x = \begin{pmatrix} T_m \tilde{x} + \tilde{H}_m J_m \tilde{x} \\ \tilde{H}_m^T \tilde{x} + T_m J_m \tilde{x} \end{pmatrix} = \begin{pmatrix} (T_m + \tilde{H}_m J_m) \tilde{x} \\ (\tilde{H}_m^T J_m + T_m) J_m \tilde{x} \end{pmatrix} = \lambda \begin{pmatrix} \tilde{x} \\ J_m \tilde{x} \end{pmatrix} = \lambda x. \quad (1)$$

The second equation $(\tilde{H}_m^T J_m + T_m) J_m \tilde{x} = \lambda J_m \tilde{x}$ of (1) is equivalent to

$$(J_m \tilde{H}_m^T + J_m T_m J_m) \tilde{x} = (\tilde{H}_m J_m + T_m) \tilde{x} = \lambda \tilde{x},$$

and therefore x is a symmetric eigenvector of T_n if and only if $\tilde{x} = x(1 : m)$ is an eigenvector of

$$(T_m + \tilde{H}_m J_m) \tilde{x} = \lambda \tilde{x}. \quad (2)$$

Similarly x is a skew-symmetric eigenvector of T_n if and only if $\tilde{x} = x(1 : m)$ is an eigenvector of

$$(T_m - \tilde{H}_m J_m) \tilde{x} = \lambda \tilde{x}. \quad (3)$$

Hence the eigenvalue problem $T_n x = \lambda x$ has been reduced to two eigenvalue problems of dimension $m = n/2$. If $n = 2m + 1$ is odd then in an analogous way the eigenvalue problem can be reduced to two eigenproblems of dimensions m and $m + 1$.

Andrew [2] and Cantoni and Butler [3] derived (2) and (3) and the corresponding equations for odd dimension n but they did not specify methods for the solution of these problems. Trench [24] applied the methods from [23] to problems (2) and (3) taking advantage of the fact that $H_m := \tilde{H}_m J_m$ is a Hankel matrix and employing fast algorithms for the solution of linear systems with Toeplitz-plus-Hankel matrices (cf. [10]).

In this note we consider a symmetry exploiting variant of the Lanczos method. It is well known that the accuracy of an approximation to an eigenvalue λ obtained by the Lanczos method is influenced mainly by the relative separation of λ from the other eigenvalues of T_n . The bigger the separation is the better is the approximation. Therefore to compute the smallest eigenvalue of T_n (or the lower part of the spectrum of T_n) it is often advantageous to apply the inverted Lanczos method, i.e., to determine the approximation from the projection of the eigenvalue problem $T_n^{-1} x = \lambda^{-1} x$ to the Krylov space $\mathcal{K}_k(T_n^{-1}, u) := \text{span}\{u, T_n^{-1}u, \dots, T_n^{-k+1}u\}$ (cf. [8,13]).

Obviously, if the initial vector u is symmetric or skew-symmetric then the whole Krylov space $\mathcal{K}_k(T_n^{-1}, u)$ belongs to the same symmetry class (and the same statement holds for $\mathcal{K}_k(T_n, u)$ or the vector spaces constructed in a rational Krylov method or in Davidson's method. Hence, the following considerations hold for these methods, too). For the restriction of T_n to the space of symmetric vectors and to skew-symmetric vectors the gaps between consecutive eigenvalues usually will be bigger than for the original matrix T_n . Thus, if the symmetry class of the principal eigenvector is known in advance then the computation of the smallest eigenvalue by the inverted Lanczos method can be accelerated by choosing the initial vector u in the appropriate symmetry class.

However, the symmetry class of the principal eigenvector is known in advance only for a small class of Toeplitz matrices. The following result was given by Trench [25]: If T_n is generated by a nonincreasing function $F : (0, \pi) \rightarrow \mathbb{R}$ and $F(0+) =: M > m := F(\pi-)$, then T_n has n distinct eigenvalues in (m, M) , its even and odd spectra are interlaced, and its largest eigenvalue is even.

In general, the smallest odd and even eigenvalues of T_n have to be determined separately, and the smaller one of them is the requested principal eigenvalue of T_n .

In section 2 we specify an algorithm which simultaneously executes the inverted Lanczos method for a symmetric and for a skew-symmetric initial vector. It is important to note that in every step only one linear system with system matrix T_n has to be solved. Moreover, for symmetry reasons the level-1-operations in the Lanczos method have to be performed only for the upper half of the vectors. Therefore, if $s \in \mathbb{R}^n$ is symmetric and $a \in \mathbb{R}^n$ is skew-symmetric then the method produces orthonormal bases of the Krylov spaces $\mathcal{K}_k(T_n^{-1}, s)$ and $\mathcal{K}_k(T_n^{-1}, a)$ essentially at the same cost as the Lanczos method for T_n and a general initial vector u . In section 3 we report on extensive numerical examples which demonstrate the favourable behaviour of the method.

2. A symmetry exploiting Lanczos method

Let $T_n := (t_{|i-j|})_{i,j=1,\dots,n}$ be a symmetric and positive definite Toeplitz matrix. The key to the simultaneous Lanczos methods with symmetric and skew-symmetric initial vectors is the following simple fact: If $v \in \mathbb{R}^n$ solves the linear system $T_n v = w$ then the symmetric part $v_s := 0.5(v + J_n v)$ of v solves the linear system $T_n v_s = 0.5(w + J_n w) =: w_s$, and the skew-symmetric part $v_a := v - v_s$ solves the linear system $T_n v_a = w - w_s$. This observation leads to the following basic form of the

Symmetry exploiting Lanczos iteration.

Let $p_1 = J p_1 \neq 0$, $q_1 = -J q_1 \neq 0$ be given initial vectors.

Set $\beta_0 = \delta_0 = 0$; $p_0 = q_0 = 0$;

$p_1 = p_1 / \|p_1\|$; $q_1 = q_1 / \|q_1\|$;

for $k = 1, 2, \dots$ until convergence do

$w = p_k + q_k$;

solve $T_n v = w$ for v ;

$v_s = 0.5 * (v + J_n v)$;

$v_a = 0.5 * (v - J_n v)$;

$\alpha_k = v'_s * p_k$;

$\gamma_k = v'_a * q_k$;

$v_s = v_s - \alpha_k * p_k - \beta_{k-1} * p_{k-1}$;

$v_a = v_a - \gamma_k * q_k - \delta_{k-1} * q_{k-1}$;

$\beta_k = \|v_s\|$;

$\delta_k = \|v_a\|$;

$p_{k+1} = v_s / \beta_k$;

$q_{k+1} = v_a / \delta_k$;

end

The iteration on the left is exactly the Lanczos method for T_n with the symmetric initial vector p_1 , and on the right we have the Lanczos method with the skew-symmetric initial vector q_1 . Selective or even full re-orthogonalization could be incorporated on either side. However, since we are interested in the smallest eigenvalue of T_n only and since for the inverted Lanczos method this eigenvalue can be expected to converge first re-orthogonalization is not necessary. This consideration is supported by the large number of examples that we considered and on which we report in section 3.

The symmetry exploiting Lanczos iteration simultaneously determines orthogonal matrices $P_k := [p_1, p_2, \dots, p_k]$ and $Q_k := [q_1, q_2, \dots, q_k]$ and two tridiagonal matrices

$$S_k := \begin{pmatrix} \alpha_1 & \beta_1 & & 0 \\ \beta_1 & \ddots & \ddots & \\ & \ddots & \ddots & \beta_{k-1} \\ 0 & & \beta_{k-1} & \alpha_k \end{pmatrix} \quad \text{and} \quad A_k := \begin{pmatrix} \gamma_1 & \delta_1 & & 0 \\ \delta_1 & \ddots & \ddots & \\ & \ddots & \ddots & \delta_{k-1} \\ 0 & & \delta_{k-1} & \gamma_k \end{pmatrix},$$

where $S_k = P_k^T T_n^{-1} P_k$ and $A_k = Q_k^T T_n^{-1} Q_k$ is the orthogonal projection of T_n^{-1} to the Krylov spaces $\mathcal{K}_k(T_n^{-1}, p_1)$ and $\mathcal{K}_k(T_n^{-1}, q_1)$, respectively. Hence the eigenvalues of S_k and A_k are the Ritz values approximating the even and odd eigenvalues of T_n^{-1} .

If $v_s =: 1/\mu_s$ is the maximal eigenvalue of S_k with corresponding normalized eigenvector y then it is well known (cf. [7, p. 364]) that there exists an eigenvalue

$\kappa =: 1/\lambda$ of T_n^{-1} such that

$$|v_s - \kappa| \leq |\beta_k y_k|, \quad (4)$$

i.e.,

$$\frac{|\lambda - \mu_s|}{\lambda} \leq |\mu_s \beta_k y_k| =: \rho_s. \quad (5)$$

Likewise if $v_a =: 1/\mu_a$ is the maximal eigenvalue of A_k and z denotes a normalized eigenvector corresponding to v_a then there exists an eigenvalue $\kappa =: 1/\lambda$ of T_n^{-1} such that

$$\frac{|\lambda - \mu_a|}{\lambda} \leq |\mu_a \delta_k z_k| =: \rho_a. \quad (6)$$

Hence, each of the intervals $[\mu_s - \sigma_s, \mu_s + \sigma_s]$, $\sigma_s := \rho_s \mu_s / (1 - \rho_s)$, and $[\mu_a - \sigma_a, \mu_a + \sigma_a]$, $\sigma_a := \rho_a \mu_a / (1 - \rho_a)$, contains at least one eigenvalue of T_n . In all of our examples $\mu := \min\{\mu_s - \sigma_s, \mu_a - \sigma_a\}$ was a lower bound of the minimum eigenvalue of T_n . However, this is not necessarily the case depending on the minimum of the angles between the eigenvector of T_n corresponding to the minimum eigenvalue and the initial vectors p_1 and q_1 . To be on the safe side one may determine the Schur parameters of $T_n - \mu I_n$ by Durbin's algorithm after the method terminated.

Each of the vectors v_s and p_k on the right of the algorithm is symmetric and each of the vectors v_a and q_k is skew-symmetric. Hence, the level-1-operations in the body of the symmetry exploiting Lanczos iteration can be performed for the upper half of the vectors only, and the following procedure results.

Let $[1; t]$, $t \in \mathbb{R}^{n-1}$, be the first column of the symmetric and positive definite Toeplitz matrix T_n of even dimension $n = 2m$. The following MATLAB function `[la,k]=seli(t,m,tol)` determines an approximation to the smallest eigenvalue of T_n such that the relative error is smaller than `tol`; k is the dimension of the Krylov space that is needed to obtain this accuracy. A MATLAB function `v=solve_toeplitz(t,n,w)` which yields the solution v of $T_n v = w$ is used.

```
function [la,k]=seli(t,m,tol);
p=rand(m,1);      q=rand(m,1);
p=p/sqrt(2*p'*p);  q=q/sqrt(2*q'*q);
err=1; k=0;
while err > tol
    k=k+1;
    w(1:m)=q+p;    w(m+1:n)=flipud(p-q);
    v=solve_toeplitz(t,n,w);
    vs=0.5*(z(1:m)+flipud(z(m+1:n))); va=z(1:m)-vs;
    ms(k,k)=2*vs'*p;      ma(k,k)=2*va'*q;
    vs=vs-ms(k,k)*p;      va=va-ma(k,k)*q;
    if k>1
        vs=vs-ms(k,k-1)*p_old;      va=va-ma(k,k-1)*q_old;
    end
end
```

```

[evs, las]=eig(ms);           [eva, laa]=eig(ma);
[las, is]=sort(diag(las));    [laa, ia]=sort(diag(laa));
ms(k,k+1)=sqrt(2*vs'*vs);    ma(k,k+1)=sqrt(2*va'*va);
ms(k+1,k)=ms(k,k+1);        ma(k+1,k)=ma(k,k+1);
if laa(k) < las(k)
    err=abs(ms(k+1,k)*evs(k,is(k)))/las(k);
else
    err=abs(ma(k+1,k)*eva(k,ia(k)))/laa(k); end
p_old=p;          q_old=q;
p=vs/ms(k+1,k);  q=va/ma(k+1,k);
end;
la=min(1/las(k), 1/laa(k));

```

The modifications for Toeplitz matrices of odd dimension $n = 2m + 1$ are obvious.

3. Numerical considerations

The most costly step in the algorithms of section 2 is the solution of the linear system

$$T_n v = w. \quad (7)$$

Equation (7) can be solved efficiently by fast or even superfast solvers (cf., e.g., [1,6,9, 15,22]) requiring $O(n^2)$ and $O(n(\log n)^2)$ flops, respectively.

In our numerical examples we solved equation (7) by the Levinson–Durbin algorithm. Durbin’s method for the corresponding Yule–Walker system supplies a decomposition $LT_n L^T = D$, where L is a lower triangular matrix and D is a diagonal matrix. Hence, in every iteration step the solution of equation (7) requires $2n^2$ flops.

For large dimensions n equation (7) can be solved using the Gohberg–Semencul formula for the inverse T_n^{-1} (cf. [9])

$$T_n^{-1} = \frac{1}{1 - y^T t} (GG^T - HH^T), \quad (8)$$

where

$$G := \begin{pmatrix} 1 & 0 & 0 & \dots & 0 \\ y_1 & 1 & 0 & \dots & 0 \\ y_2 & y_1 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ y_{n-1} & y_{n-2} & y_{n-3} & \dots & 1 \end{pmatrix} \quad \text{and} \quad H := \begin{pmatrix} 0 & 0 & 0 & \dots & 0 \\ y_{n-1} & 0 & 0 & \dots & 0 \\ y_{n-2} & y_{n-1} & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ y_1 & y_2 & y_3 & \dots & 0 \end{pmatrix}$$

are Toeplitz matrices and y denotes the solution of the Yule–Walker system $T_{n-1}y = t$.

The advantages associated with equation (8) are at hand. Firstly, the representation of the inverse of T_n requires only n storage elements. Secondly, the matrices G , G^T , H and H^T are Toeplitz matrices, and hence the solution $T_n^{-1}w$ can be calculated in only

Table 1
Average number of flops and iteration steps.

dim	Lanczos method			SELI		
	flops		steps	flops		steps
32	3.68E4	(1.13E5)	7.53	2.78E4	(8.60E4)	5.73
64	1.02E5	(4.39E5)	8.00	8.00E4	(3.39E5)	6.15
128	3.27E5	(9.39E5)	7.95	2.51E5	(7.04E5)	5.89
256	1.28E6	(2.17E6)	8.35	9.67E5	(1.62E6)	6.07
512	5.20E6	(5.11E6)	8.73	3.83E6	(3.77E6)	6.16
1024	2.16E7	(1.25E7)	9.24	1.58E7	(9.38E6)	6.45

$O(n \log n)$ flops using the fast Fourier transform. Experiments show that for $n \geq 512$ this approach is actually more efficient than the Levinson–Durbin algorithm.

To test the improvement of the symmetry exploiting Lanczos iteration upon the ordinary Lanczos method we considered Toeplitz matrices

$$T = \xi \sum_{j=1}^n \eta_j T_{2\pi\theta_j}, \quad (9)$$

where ξ is chosen such that the diagonal of T is normalized to 1, η_j and θ_j are uniformly distributed random numbers in the interval $[0, 1]$ and $T_\theta = (\cos(\theta(i - j)))_{i,j=1,\dots,n}$ (cf. [4]).

For each of the dimensions $n = 32, 64, 128, 256, 512$ and 1024 we considered 100 test examples. Table 1 contains the average number of flops and the average dimension k of the Krylov spaces needed to determine an approximation to the smallest eigenvalue with relative error less than 10^{-6} . Here we solved the linear systems using the Levinson–Durbin algorithm. In parenthesis we added the average number of flops using the Gohberg–Semencul formula.

Huckle [13] suggested to use the error estimate corresponding to (4) after a small number of steps of the inverted Lanczos process to obtain a good lower bound σ of the smallest eigenvalue of T_n and to continue with the spectral transformation Lanczos method with this shift, i.e., the Lanczos method for $(T_n - \sigma I_n)^{-1}$. Obviously, Huckle’s approach can be combined with the symmetry exploiting Lanczos method considered here. However, the example above demonstrates that after a very small number of Lanczos steps a good approximation of the smallest eigenvalue is derived. Hence, the variant of Huckle usually will not pay, at least for the class of Toeplitz matrices considered here.

4. Concluding remarks

In this note we presented a symmetry exploiting variant of the inverted Lanczos method to determine the smallest eigenvalue of a real symmetric and positive definite

Toeplitz matrix which improves the classical Lanczos method considerably. In the numerical examples we solved Toeplitz systems by the Levinson–Durbin algorithm or by the Gohberg–Semencul formula. Superfast Toeplitz solvers can be incorporated as well reducing the complexity of the method to $O(n(\log n)^2)$.

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