A Method of Order $1+\sqrt{3}$ for Computing the Smallest Eigenvalue of a Symmetric Toeplitz Matrix

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Abstract: In this note we discuss a method of order $1+\sqrt{3}$ for computing the smallest eigenvalue λ_1 of a symmetric and positive definite Toeplitz matrix. It generalizes and improves a method introduced in [7] which is based on rational Hermitean interpolation of the secular equation. Taking advantage of a further rational approximation of the secular equation which is essentially for free and which yields lower bounds of λ_1 we obtain an improved stopping criterion.

Keywords: eigenvalue problem, Toeplitz matrix, secular equation

1 Introduction

The problem of finding the smallest eigenvalue λ_1 of a real symmetric, positive definite Toeplitz matrix T is of considerable interest in signal processing. Given the covariance sequence of the observed data, Pisarenko [11] suggested a method which determines the sinusoidal frequencies from the eigenvector of the covariance matrix associated with its minimum eigenvalue. The computation of the minimum eigenvalue of T was studied in, e.g. [1], [4], [5], [6], [7], [8], [9], [10], [12], [13], [14].

In their seminal paper [1] Cybenko and Van Loan presented the following method: By bisection they first determine an initial approximation $\mu_0 \in (\lambda_1, \omega_1)$ where ω_1 denotes the smallest pole of the secular equation f, and they improve μ_0 by Newton's method for f which converges monotonely and quadratically to λ_1. By replacing Newton's method by a root finding method based on Rational Hermitean interpolation of f Mackens and the second author in [7] improved this approach substantially.

In this note we revisit this method. In [7] the k-th iterate μ_k was chosen to be the unique root of

$$g(\lambda) = a_0 + a_1(\lambda-\alpha) + (\lambda-\alpha)^2 \frac{b}{c-\lambda}$$

in (α, μ_{k-1}) where α is a lower bound of λ_1 obtained in the bisection phase, and a_0, a_1, b and c are chosen such that g interpolates f at α and μ_{k-1} in the Hermitean sense. It was proved that this method converges monotonely and quadratically to λ_1 and that it converges faster than Newton's method, i.e. if $\mu \in (\lambda_1, \omega_1)$ then the smallest root of g is closer to λ_1 than the Newton iterate with initial guess μ.

The method suffers the same disadvantage as the method of false position for convex or concave functions: one interpolation knot (in our case α) is stationary, and only the other one converges momotonely to the wanted solution. In the root finding case one gains a substantial improvement if one drops the requirement that f has opposite signs at the two interpolation knots and replaces the method of false position by the secant method. In this note we prove that the method in [7] can be improved in a similar way if one chooses the new iterate μ_k as the unique root of g were the parameters a_0, a_1, b and c are determined such that g and g' interpolate f and f', respectively, at μ_k and μ_{k-1}. It is shown that the order of convergence of this modified method is $1+\sqrt{3}$.

In [7] we based a stopping criterion on a lower bounds of λ_1 which are determined from a quadratic interpolation. This one is improved using a further rational interpolation of f with a fixed pole which is obtained for free in the course of the algorithm.

2 Rational Hermitean interpolation

Let $T \in \mathbb{R}^{(n,n)}$ be a symmetric positive definite Toeplitz matrix. We assume that its diagonal is normalized and consider the following partition:

$$T = \begin{pmatrix} 1 & t^T \\ t & G \end{pmatrix}.$$

It is well known that the eigenvalues of T and of G are real and positive and satisfy the interlacing property $\lambda_1 \leq \omega_1 \leq \lambda_2 \leq \ldots \leq \omega_{n-1} \leq \lambda_n$ where λ_j and ω_j is the jth smallest eigenvalue of T and its principal submatrix G, respectively.

We assume that $\lambda_1 < \omega_1$. Then λ_1 is the smallest root of the secular equation

$$f(\lambda) := -1 + \lambda + t^T(G - \lambda I)^{-1}t = 0. \qquad (1)$$

It is easily seen that f is strictly monotonely increasing and strictly convex in the interval $(0, \omega_1)$, and therefore for every initial value $\mu_0 \in (\lambda_1, \omega_1)$ Newton's method converges monotonely decreasing and quadratically to λ_1.

Cybenko and Van Loan [1] suggested to determine an initial value μ_0 by bisection based on Durbin's algorithm (cf. [2], p. 184 ff). If μ is not in the spectrum of any of the principal submatrices of $T - \mu I$ then Durbin's algorithm applied to $(T - \mu I)/(1 - \mu)$ determines a lower triangular matrix

$$L = \begin{pmatrix} 1 & 0 & \ldots & 0 \\ \ell_{21} & 1 & \ldots & 0 \\ \vdots & \vdots & \ddots & \\ \ell_{n1} & \ell_{n2} & \ldots & 1 \end{pmatrix}$$

such that

$$\frac{1}{1-\mu} L(T - \mu I)L^T = D := \mathrm{diag}\{1, E_1, \ldots, E_{n-1}\}. \qquad (2)$$

If $\tilde{L}$ is obtained from L by dropping the last row and last column then obviously

$$\frac{1}{1-\mu} \tilde{L}(G - \mu I)\tilde{L}^T = \tilde{D} := \mathrm{diag}\{1, E_1, \ldots, E_{n-2}\}$$

Hence, from Sylvester's law of inertia one gets

(i) $\mu < \lambda_1$, if $E_j > 0$ for $j = 1, \ldots, n-1$,

(ii) $\mu \in [\lambda_1, \omega_1)$, if $E_j > 0$ for $j = 1, \ldots, n-2$ and $E_{n-1} \leq 0$,

(iii) and $\mu > \omega_1$, if $E_j < 0$ for some $j \in \{1, \ldots, n-2\}$.

An upper bound of λ_1 to start the bisection process can be obtained in the following way. Let $w := -G^{-1}t$ be the solution of the Yule–Walker system. Then

$$q := \frac{1}{1 + t^T w} \begin{pmatrix} 1 \\ w \end{pmatrix} = T^{-1}e^1$$

is the first iterate of the inverse iteration with shift parameter 0 starting with the unit vector e_1 which can be expected to be not too bad an approximation of the eigenvector corresponding to the smallest eigenvalue λ_1. The Rayleigh quotient

$$R(q) := \frac{q^T T q}{q^T q} = \frac{1 + t^T w}{1 + \|w\|_2^2} \qquad (3)$$

is an upper bound of λ_1 which should be not too bad either.

Since

$$f'(\lambda) = 1 + \|(G - \lambda I)^{-1}t\|_2^2, \qquad (4)$$

a Newton step can be performed in the following way:

$$\text{Solve } (G - \mu_k I)w = -t \quad \text{for} \quad w,$$
$$\text{and set } \mu_{k+1} := \mu_k - \frac{-1 + \mu_k - w^T t}{1 + \|w\|_2^2}$$

where the Yule-Walker system

$$(G - \mu I)w = -t \qquad (5)$$

can be solved by Durbin's algorithm requiring $2n^2$ flops.

The global convergence behaviour of Newton's method usually is not satisfactory since the smallest root λ_1 and the smallest pole ω_1 of the rational function f can be very close to each other. In this situation the initial steps of Newton's method are extremely slow, at least if the initial guess is close to ω_1.

Approximating the secular equation by a suitable rational function the convergence of the method (i.e. the bisection phase and the root finding by

Newton's method) can be improved considerably. In terms of condensation methods (cf. [3]) the secular equation f can be interpreted as the exact condensation of the eigenvalue problem $Tx = \lambda x$ where $x_2, \dots, x_n$ are chosen to be slaves and x_1 is the only master. Using spectral information of the slave problem $(G - \mu I)v = 0$ the function f obtains the form (cf. [3])

$$f(\lambda) = f(0) + f'(0)\lambda + \lambda^2 \sum_{j=1}^{n-1} \frac{\alpha_j^2}{\omega_j - \lambda},$$

where α_j, $j = 1, \dots, n-1$, are real numbers depending on the eigenvectors of G. With a shift μ which is not in the spectrum of G f can be rewritten as

$$f(\lambda) = f(\mu) + (\lambda - \mu)f'(\mu) + (\lambda - \mu)^2\phi(\lambda;\mu) \quad (6)$$

where

$$\phi(\lambda;\mu) = \sum_{j=1}^{n-1} \frac{\alpha_j^2\gamma_j^2}{\omega_j - \lambda}, \quad \gamma_j = \frac{\omega_j}{\omega_j - \mu}. \quad (7)$$

The representation (6) and (7) of f suggests to replace the linearization of f in Newton's method by a root finding method based on a rational model

$$g(\lambda;\mu,\nu) = f(\mu) + (\lambda-\mu)f'(\mu) + (\lambda-\mu)^2 \frac{b}{c - \lambda}, \quad (8)$$

where μ and ν are given approximations to λ_1 and b and c are determined such that

$$g(\nu;\mu,\nu) = f(\nu),\ g'(\nu;\mu,\nu) = f'(\nu). \quad (9)$$

Theorem 1: *Let g be given by (8) and (9) where μ and ν are not in the spectrum of G. Then*

$$b = \frac{\phi(\nu;\mu)^2}{\phi'(\nu;\mu)} \geq 0,\ c = \nu + \frac{\phi(\nu;\mu)}{\phi'(\nu;\mu)} \geq \omega_1. \quad (10)$$

Proof: From equations (6) and (8) we obtain

$$g(\lambda;\mu,\nu) - f(\lambda) = (\lambda - \mu)^2 \left(\frac{b}{c - \lambda} - \phi(\lambda;\mu) \right). \quad (11)$$

Hence the interpolation conditions (9) yield

$$\frac{b}{c - \nu} - \phi(\nu;\mu) = 0,\ \frac{b}{(c - \nu)^2} - \phi'(\nu;\mu) = 0,$$

from which we get the representations of b and c in (10).

$b \geq 0$ is obvious, and $c \geq \omega_1$ follows from

$$c = \sum_{j=1}^{n-1} \frac{\alpha_j^2\gamma_j^2}{(\omega_j - \nu)^2}\omega_j \Bigg/ \sum_{j=1}^{n-1} \frac{\alpha_j^2\gamma_j^2}{(\omega_j - \nu)^2}$$

which is obtained from (7) and (10). □

Theorem 2: *If μ and ν are not in the spectrum of G it holds*

$$f(\lambda) - g(\lambda) = (\lambda - \mu)^2(\lambda - \nu)^2\psi(\lambda;\mu,\nu) \quad (12)$$

where $\psi = \psi_1/\psi_2$,

$$\psi_1 = \sum_{1 \leq j < k \leq n-1} \frac{\alpha_j^2\alpha_k^2\omega_j^2\omega_k^2(\omega_k - \omega_j)^2}{\tau_{jk}(\mu)^2\tau_{jk}(\nu)^2(\omega_j - \lambda)(\omega_k - \lambda)},$$

$$\tau_{jk}(\lambda) = (\omega_j - \lambda)(\omega_k - \lambda)$$

and

$$\psi_2 = \sum_{j=1}^{n-1} \frac{\alpha_j^2\omega_j^2}{(\omega_j - \mu)^2(\omega_j - \nu)^2}(\omega_j - \lambda).$$

Proof: From equations (10) and (11) it follows

$$f(\lambda) - g(\lambda) = (\lambda - \mu)^2 \left(\phi(\lambda;\mu) - \frac{\phi(\nu;\mu)^2}{\phi(\nu;\mu) + (\nu - \lambda)\phi'(\nu;\mu)} \right),$$

and taking advantage of (7) an easy but lengthy calculation yields (12). □

In particular we obtain from Theorem 2 $g(\lambda_1) < 0$, and since g is strictly monotonely increasing and strictly convex in $[0, c) \supset [0, \omega_1)$ and $\lim_{\lambda \uparrow c} g(\lambda;\mu,\nu) = \infty$ the unique root of g in $[0, c)$ is an upper bound of the smallest eigenvalue λ_1 of T.

Assume that we are given a lower bound μ_0 of λ_1 and an upper bound $\mu_1 \in (\lambda_1, \omega_1)$ which is obtained by bisection, e.g. Then the unique root μ_2 of $g(\cdot;\mu_1,\mu_0)$ in $(0, c)$ satisfies $\lambda_1 \leq \mu_2 < \mu_1$. Mackens and the second author in [7] considered a method of false position like iteration where μ_{k+1} is defined as the unique root of $g(\cdot;\mu_k,\mu_0)$, and they proved this method to be quadratically convergent.

Here we study the method which corresponds to the secant method where μ_{k+1} is determined as the unique root of $g(\cdot;\mu_k,\mu_{k-1})$. Again this algorithm yields a monotonely decreasing sequence $\{\mu_k\}$ which is bounded below by λ_1. The following Theorem 3 proves the convergence of this sequence to λ_1 and its order of convergence $1 + \sqrt{3}$.

Theorem 3: *Let $\mu_1 \in (\lambda_1, \omega_1)$ and for $k \geq 2$ let μ_{k+1} be the unique root of $g(\cdot;\mu_k,\mu_{k-1})$ in $[0, \omega_1)$.*

Then the sequence $\{\mu_k\}$ converges monotonely decreasing to λ_1, and its R-order of convergence is $1+\sqrt{3}$.

Proof: Let $\epsilon_k := \mu_k - \lambda_1$. From $g(\mu_{k+1};\mu_k,\mu_{k-1}) = 0$ and Theorem 2 we obtain for some $\xi_k \in (\lambda_1, \mu_{k+1})$

$$f(\mu_{k+1}) - f(\lambda_1) = f'(\xi_k)\epsilon_{k+1} = (\mu_k - \mu_{k+1})^2(\mu_{k-1} - \mu_{k+1})^2\psi(\mu_{k+1},\mu_k,\mu_{k-1}).$$

The sequence $\{\mu_k\}$ is monotonely decreasing and bounded away from ω_1. Hence there exists $C > 0$ such that

$$\epsilon_{k+1} \le C\epsilon_k^2\epsilon_{k-1}^2,$$

and for $e_k := C^{1/3}\epsilon_k$ it holds

$$e_{k+1} \le e_k^2 e_{k-1}^2.$$

Let $p = 1+\sqrt{3}$ and $\eta := \min(e_0, e_1^{1/p})$. We prove by induction

$$e_k \le \eta^{(p^k)} \tag{13}$$

which demonstrates that the R-order of convergence of μ_k equals $1+\sqrt{3}$.

For $k=0$ and $k=1$ (13) is trivial. If it hold for integers up to k then it follows from $2(1+p) = p^2$

$$\begin{aligned} e_{k+1} &\le e_k^2 e_{k-1}^2 \le \eta^{(2p^k)}\eta^{(2p^{k-1})} \\ &= \eta^{(2(1+p)p^{k-1})} = \eta^{(p^{k+1})}. \ \square \end{aligned}$$

With a further rational interpolation of the secular equation we are able to construct a lower bound of λ_1. This will be the basis of our stopping criterion.

Theorem 4: *Let $\kappa \in (0,\lambda_1)$, $\mu \in (\kappa,\omega_1)$ and $p \in (\kappa,\omega_1)$. Let*

$$h(\lambda) := f(\mu) + f'(\mu)(\lambda-\mu) + (\lambda-\mu)^2\frac{b}{p-\lambda},$$

where b is determined such that the interpolation condition $h(\kappa) = f(\kappa)$ holds.

Then $b > 0$, i.e. h is strictly monotonely increasing and strictly convex in $(0,p)$, and the unique root of h in $(0,p)$ is a lower bound of λ_1.

Proof: From equation (6) and from the interpolation condition $h(\kappa) = f(\kappa)$ we obtain

$$b = (p-\kappa)\phi(\kappa;\mu) > 0.$$

That the unique root $\tilde{\lambda}$ of h in $(0,p)$ is a lower bound of λ_1 is obvious for $p \le \lambda_1$. For $p > \lambda_1$ we have to show $h(\lambda_1) > 0$. This follows from equations (6) and (7):

$$\begin{aligned} h(\lambda_1) &= f(\mu) + f'(\mu)(\lambda_1-\mu) + (\lambda_1-\mu)^2\frac{b}{p-\lambda_1} \\ &= f(\lambda_1) - (\lambda_1-\mu)^2\left(\phi(\lambda_1) - \frac{(p-\kappa)\phi(\kappa)}{p-\lambda_1}\right) \\ &= \frac{(\lambda_1-\mu)^2}{p-\lambda_1}\left((p-\kappa)\phi(\kappa) - (p-\lambda_1)\phi(\lambda_1)\right) \\ &= \frac{(\lambda_1-\mu)^2}{p-\lambda_1}\sum_{j=1}^{n-1}\gamma_j^2\left(\frac{p-\kappa}{\omega_j-\kappa} - \frac{p-\lambda_1}{\omega_j-\lambda_1}\right) \\ &= \frac{(\lambda_1-\mu)^2}{p-\lambda_1}\sum_{j=1}^{n-1}\gamma_j^2\frac{(\omega_j-p)(\lambda_1-\kappa)}{(\omega_j-\kappa)(\omega_j-\lambda_1)} > 0. \quad \square \end{aligned}$$

Theorem 4 can be used to construct lower bounds of λ_1 in the course of the algorithm which are essentially for free. We already pointed out that Durbin's algorithm determines the factorization of $T - \mu I$ given in (2). Hence, solving the Yule–Walker system for some μ we can evaluate the characteristic polynomial

$$\chi(\mu) = (1-\mu)E_1 \cdot \ldots \cdot E_{n-2}$$

of G at negligible cost. Moreover, $\chi(\lambda)$ (or $-\chi(\lambda)$) is monotonely decreasing and convex for $\lambda \le \omega_1$. Therefore, if $\chi(\mu_1)$ and $\chi(\mu_2)$ are known for $\mu_1,\mu_2 \in [0,\omega_1)$ then a secant step for χ yields an improved lower bound of ω_1.

3 A MATLAB progam

The following MATLAB program determines a lower bound μ of the smallest eigenvalue of a symmetric and positive definite Toeplitz matrix which is given by the vector t of dimension n. It uses the function `[f,Df,chi,loc]=durbin(mu,t,n)` which returns the value `f` of the secular equation at μ, its derivative `Df`, the value `chi` of the characteristic polynomial of G, and the location

$$\texttt{loc} = \begin{cases} 0 & \text{if} \quad \mu < \lambda_1 \\ 1 & \text{if} \quad \lambda_1 \le \mu < \omega_1 \\ 2 & \text{if} \quad \mu > \omega_1 \end{cases}$$

of `mu` within the spectrum of T.

The functions `rat_app` and `rat_app_fp` return the smallest positive root of the rational function g and h, respectively.

```
 1 function mu=toeplitz_ev(t,n,tol)
 2 [f0,Df0,chi0,loc]=durbin(0,t,n);
 3 mu0=0; p=0;
 4 lb=0; ub=-f0/Df0;
 5 ka=0; fka=f0;
 6 mu=rand*ub;
 7 rel_err=1;
 8 while abs(rel_err) > tol
 9   [f,Df,chi,loc]=durbin(mu,t,n);
10   if loc == 2
11     lambda=rat_app(mu0,f0,Df0,mu,f,Df);
12     ub=min([mu,ub,lambda]);
13     mu=0.5*(lb+ub);
14   else
15     p=max(p,mu-(mu-mu0)*chi/(chi-chi0));
16     lb=rat_app_fp(ka,fka,mu,f,Df,p);
17     root=rat_app(mu0,f0,Df0,mu,f,Df));
18     ub=min(ub,root);
19     mu0=mu;f0=f;Df0=Df;chi0=chi;
20     if loc == 0
21       ka=mu0;fka=f0;end
22     rel_err=ub/lb-1;
23     if loc == 1
24       mu=root;
25     else
26       newt=mu-f0/Df0;
27       if abs((root-newt)/root)<0.01
28         mu=root;
29       else
30         mu=0.1*lb+0.9*ub;
31         end
32       end
33     end
34   end
```

Some remarks are in order.

2 – 3 : mu0< λ_1 with known f0= f(mu0), Df0= f'(mu0) and chi0= χ(mu0) is one knot in the rational interpolation of f and the secant method for χ. p is a lower bound of ω_1 used to determine a lower bound of λ_1.

4 : lb is a lower bound of λ_1 and ub an upper bound. ub=-s0/Ds0 is obtained from (6).

5 : ka is a lower bound of λ_1 with known fka= f(ka) which corresponds to κ in Theorem 4.

6 : The algorithm starts with a test parameter mu randomly chosen in the interval [lb,ub].

10 – 13 : By Theorem 2 the smallest root lambda of $g(\cdot;$mu$,$mu0$)$ is an upper bound of λ_1. It is for free, and in some cases it is smaller than mu. This modification of the bisection method actually improves the performance of the method.

15 : The lower bound p of the pole might be improved by a secant step for the characteristic polynomial of G.

16 : lb is the lower bound of λ_1 from Theorem 4.

17 – 18 : The root of $g(\cdot;$mu$,$mu0$)$ is an upper bound of λ_1, and it further enhances the bisection method.

20 – 21 : If mu< λ_1, mu can be used as κ of Theorem 4 in subsequent iteration steps.

23 – 24 : For mu$\in (\lambda_1, \omega_1)$ the method continues with test parameter mu=root.

25 – 32 : For mu< λ_1 we introduce a tie break rule which was motivated in [7]. newt is the result of a Newton step for f. Hence root and newt are second order approximations of λ_1. If they are not close to each other the test parameter mu can not be close to λ_1. In this case we reduce the next test parameter. This modification improves the performance of the method, in particular if the gap between λ_1 and ω_1 is very narrow.

4 Numerical results

To test the method we considered the following class of Toeplitz matrices:

$$T = m \sum_{k=1}^{n} \eta_k T_{2\pi\theta_k}, \tag{14}$$

where m is chosen such that the diagonal of T is normalized to $t_0 = 1$,

$$T_\theta = (T_{ij}) = (cos(\theta(i-j))),$$

and η_k and θ_k are uniformly distributed random numbers in the interval $[0, 1]$ (cf. Cybenko and Van Loan [1]).

Table 1 contains the average number of flops and the average number of Durbin steps needed to determine the smallest eigenvalue in 100 test problems with each of the dimensions $n = 32$, 64, 128, 256, 512, 1024 and 2048. The iteration was terminated if the error was guaranteed to be less than 10^{-6} by the error bound from Theorem 4. For comparison we added the results for the quadratically convergent method in [7].

dim.	order $1+\sqrt{3}$		method in [7]	
	flops	steps	flops	steps
32	1.086 $E04$	4.34	1.153 $E04$	4.67
64	4.639 $E04$	5.14	4.669 $E04$	5.39
128	1.804 $E05$	5.25	1.900 $E05$	5.79
256	7.837 $E05$	5.84	8.790 $E05$	6.85
512	3.512 $E06$	6.62	3.892 $E06$	7.69
1024	1.531 $E07$	7.26	1.730 $E07$	8.75
2048	6.268 $E07$	7.45	7.590 $E07$	9.59

Tab. 1.

5 Concluding Remarks

We have presented an algorithm for computing the smallest eigenvalue of a symmetric and positive definite Toeplitz matrix of order $1+\sqrt{3}$. Realistic error bounds were obtained at negligible cost. We used Durbin's algorithm to solve the occuring Yule–Walker systems and to determine the Schur parameters E_j requiring $2n^2$ flops. This information can be gained from superfast Toeplitz solvers the complexity of which is only $O(n \log^2 n)$ operations. In a similar way as in [12] or [13] the method can be enhanced taking advantage of symmetry properties of the eigenvectors of T.

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