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 $\lambda_1 \le \omega_1 \le \lambda_2 \le \ldots \le \omega_{n-1} \le \lambda_n$ 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 $E_{n-1} \le 0$,

(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 $x_2, \ldots, x_n$ 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, $j = 1, \ldots, n-1$, 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). $\square$

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). $\square$

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`$<\lambda_1$ with known `f0`$=f($`mu0`$)$, `Df0`$=f'($`mu0`$)$ and `chi0`$=\chi($`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`$<\lambda_1$, `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`$<\lambda_1$ 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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