# A New Acceleration of the Projection Method in Nonsymmetric Eigenvalue Problems

A. Nishida and Y. Oyanagi

Department of Information Science
University of Tokyo
Tokyo, Japan 113

## Abstract

*This study proposes a new method for the acceleration of the projection method to compute a few eigenvalues with the largest real parts of a large nonsymmetric matrix.*

*In the field of the solution of the linear system, an acceleration using the least squares polynomial which minimizes its norm on the boundary of the convex hull formed with the unwanted eigenvalues are proposed. We simplify this method for the eigenvalue problem using the same property of the orthogonal polynomial. This study applies the Tchebychev polynomial to the iterative Arnoldi method and proves that the new method computes necessary eigenvalues with far less complexity than the QR method. Its high accuracy enables us to compute the close eigenvalues that can not be obtained by the simple Arnoldi method.*

## 1 Introduction

In the fluid dynamics and the structural analysis, there are a number of cases where a few eigenvalues with the largest real parts of a nonsymmetric matrix are required. In economic modeling, the stability of a model is interpreted in terms of the dominant eigenvalues of a large nonsymmetric matrix [7, 9].

Several methods have been proposed for this problem. The method proposed by Arnoldi in 1951 [1] and the subspace iteration method due to Rutishauser [5], which are variants of the projection method, have been the most effective for this purpose. The Arnoldi method, however, has a drawback of the expense of too much memory space. This problem is solved by using the method iteratively (Saad [6]). Although the iterative Arnoldi method is quite effective and may excel the subspace iteration method in performance, the dimension of the subspace is inevitably large, in particular when the wanted eigenvalues are clustered. Moreover it favors the convergence on the envelope of the spectrum.

To overcome this difficulty Saad [7] proposed a Tchebychev acceleration technique for the Arnoldi method, which is an expansion of the similar technique for symmetric matrices. In the nonsymmetric case, we have to consider the distribution of the eigenvalues in the complex plane. The normalized Tchebychev function $P_n(\lambda) = T_n(\frac{d-\lambda}{c})/T_n(\frac{d}{c})$ has the property

$$\lim_{n\to\infty} P_n(\lambda) = \begin{cases} 0 & \lambda \text{ is inside of } \hat{F}(d,c) \\ \infty & \lambda \text{ is outside of } \hat{F}(d,c) \end{cases},$$

where $d$ and $d \pm c$ are the center and the focal points of the ellipse $\hat{F}(d,c)$, which passes through the origin. Considering the optimal ellipse which encloses the unnecessary eigenvalues obtained by the previous step of the Arnoldi method and applying this polynomial to the matrix of the problem, we can make the new matrix whose necessary eigenvalues are made dominant (Manteuffel [4]). We continue the subsequent Arnoldi iterations with the new matrix. This algorithm was refined and expanded by Ho [3] to the case where the reference eigenvalues do not have the largest or the smallest real parts. However, the methods based on the optimal ellipse have a defect of making the excessively large ellipse compared with the distribution of the unwanted eigenvalues.

In this paper, we use the convex hull proposed for the solution of the nonsymmetric linear system (Saad [8]) instead of the Manteuffel's optimal ellipse. The least squares polynomials minimize the $L_2$ norm defined on the boundary of the convex hull which encloses the unnecessary eigenvalues. From the maximum modulus principle, the absolute value of the polynomial is guaranteed to take on a maximum on the boudary of the convex hull. The polynomials can

be generated without any numerical integration, using the orthogonality of the Tchebychev functions. In the eigenvalue problem, we can directly use the orthonormal polynomial generated by the Tchebychev functions as the mini-max polynomial, since we have no need to normalize the polynomial at the origin.

The numerical experiments show that the method is effective for this purpose. The iteration of the Arnoldi method proposed by Saad is used in our algorithm and contributes to the economization of the memory space, which is consumed mainly by the coefficients of the polynomials.

## 2 Background

This section gives an outline of the methods referred to in this paper. The Arnoldi method, which is a variant of the projection method, plays the main role in our problem. The principle of the acceleration technique using the optimal ellipse [4] is explained briefly, since the properties used in this method are also important in our algorithm. We then describe the Tchebychev-Arnoldi method using the optimal ellipse and the least-squares based method, which were developed for solving the linear system by Saad [7, 8].

### 2.1 The Arnoldi method

If $u \neq 0$, let $K_l = \mathrm{lin}(u, Au, \cdots, A^{l-1}u)$ be the Krylov subspace generated by $u$. Arnoldi's method computes an orthogonal basis $\{v_i\}_1^l$ of $K_l$ in which the map is represented by an upper Hessenberg matrix i.e., an upper triangular matrix with sub-diagonal elements:

1. $v_1 = u/ \parallel u \parallel_2, \quad h_{1,1} = (Av_1, v_1)$;
2. for $j = 1, \cdots, l-1$, put

$$x_{j+1} = Av_j - \sum_{i=1}^{j} h_{ij} v_i, \quad h_{j+1,j} = \parallel x_{j+1} \parallel_2,$$

$$v_{j+1} = h_{j+1}^{-1} x_{j+1}, \quad h_{i,j+1} = (Av_{j+1}, v_i)$$
$$(i \leq j+1).$$

The algorithm terminates when $x_j = 0$, which is impossible if the minimal polynomial of $A$ with respect to $u$ is of degree $\geq l$. If this condition is satisfied, $H_l = (h_{ij})$ is an irreducible Hessenberg matrix.

An iterative variant of the method is proposed by Saad [7]. Starting with an initial vector $u$ and fixing a moderate value $m$ we compute the eigenvectors of $A_m$. We begin again, using as a starting vector a linear combination of the eigenvectors. No proof exists for the convergence of this method.

### 2.2 The Tchebychev-Arnoldi method

The original idea of using the Tchebychev polynomial for filtering the desired eigenvalues was proposed by Manteuffel in 1977 [4]. It was applied to the solution of nonsymmetric linear systems.

If $x_0$ is the initial guess at the solution x, an iteration is defined with the general step $x_n = x_{n-1} + \sum_{i=1}^{n-1} \gamma_{ni} r_i$ where the $\gamma_{ij}$'s are constants and $r_i = b - Ax_i$ is the residual at step $i$. Let $e_i = x - x_i$ be the error at the $i$th step then an inductive argument yields $e_n = [I - As_n(A)]e_0 \equiv P_n(A)e_0$ where $s_n(z)$ and $P_n(z)$ are polynomials of degree $n$ such that $P_n(0) = 1$. To make $\parallel e_n \parallel \leq \parallel P_n(A) \parallel \parallel e_0 \parallel$ small, the Tchebychev polynomial is used as the sequence of polynomials.

The Tchebychev polynomials are given by $T_n(z) = \cosh(n \cosh^{-1}(z))$. Let $F(d, c)$ be the member of the family of ellipses in the complex plane centered at $d$ with the focal points at $d + c$ and $d - c$, where $d$ and $c$ are complex numbers. Suppose $z_i \in F_i(0, 1)$, $z_j \in F_j(0, 1)$; then

$$\Re(\cosh^{-1}(z_i)) < \Re(\cosh^{-1}(z_j)) \Leftrightarrow F_i(0,1) \subset F_j(0,1),$$

$$\Re(\cosh^{-1}(z_i)) = \Re(\cosh^{-1}(z_j)) \Leftrightarrow F_i(0,1) = F_j(0,1).$$

Consider the scaled and translated Tchebychev polynomials $P_n(\lambda) = T_n(\frac{d-\lambda}{c})/T_n(\frac{d}{c})$. Using the definition of the cosh, we can see that

$$P_n(\lambda) = \frac{e^{n \cosh^{-1}(\frac{d-\lambda}{c})} + e^{-n \cosh^{-1}(\frac{d-\lambda}{c})}}{e^{n \cosh^{-1}(\frac{d}{c})} + e^{-n \cosh^{-1}(\frac{d}{c})}}$$

$$\doteq e^{n \cosh^{-1}(\frac{d-\lambda}{c}) - n \cosh^{-1}(\frac{d}{c})}$$

for large $n$.

Let $r(\lambda) = \lim_{n\to\infty} |P_n(\lambda)^{\frac{1}{n}}|$, then we have

$$r(\lambda) = e^{\Re(\cosh^{-1}(\frac{d-\lambda}{c}) - \cosh^{-1}(\frac{d}{c}))}.$$

From the above lemma and the definition of $r(\lambda)$, we have that if $\lambda_i \in F_i(d, c), \lambda_j \in F_j(d, c)$, then

$$r(\lambda_i) < r(\lambda_j) \Leftrightarrow F_i(d,c) \subset F_j(d,c)$$

$$r(\lambda_i) = r(\lambda_j) \Leftrightarrow F_i(d,c) = F_j(d,c)$$

$$r(\lambda) = 1 \Leftrightarrow \lambda \in \hat{F}(d,c),$$

where $\hat{F}(d, c)$ is the member of the family passing through the origin. Thus we have

$$\lim_{n\to\infty} P_n(\lambda) = \begin{cases} 0 & \lambda \text{ is inside of } \hat{F}(d,c) \\ \infty & \lambda \text{ is outside of } \hat{F}(d,c) \end{cases}.$$

Suppose that we can find the ellipse that contains all the eigenvalues of $A$ except for the $r$ wanted ones. Then the algorithm runs a certain number of steps of the Tchebychev iteration and take the resulting vector $z_n$ as the initial vector in the Arnoldi process. From the Arnoldi purification process one obtains a set of $m$ eigenvalues, $r$ of which are the approximation to the $r$ wanted ones, while the remaining ones will be used for adaptively constructing the best ellipse.

- *Start:* Choose an initial vector $v_1$, a number of Arnoldi steps $m$ and a number of Tchebychev steps $n$.
- *Iterate:*
  1. Perform the $m$ steps of the Arnoldi algorithm starting with $v_1$. Compute the $m$ eigenvalues of the resulting Hessenberg matrix. Select the $r$ eigenvalues of the largest real parts $\tilde{\lambda}_1, \cdots, \tilde{\lambda}_r$ and take $\tilde{R} = \{\tilde{\lambda}_{r+1}, \cdots, \tilde{\lambda}_m\}$. If satisfied stop, otherwise continue.
  2. Using $\tilde{R}$, obtain the new estimates of the parameters $d$ and $c$ of the best ellipse. Then compute the initial vector $z_0$ for the Tchebychev iteration as a linear combination of the approximate eigenvectors $\tilde{u}_i, \quad i = 1, \cdots, r$.
  3. Perform $n$ steps of the Tchebychev iteration to obtain $z_n$. Take $v_1 = z_n / \parallel z_n \parallel$ and back to 1.

### 2.3 The least-squares based method

It has been shown that the least-squares based method for solving linear systems is competitive with the ellipse based methods and are more reliable (Saad [8]).

By the maximum principle, the maximum modulus of $|1 - \lambda s_n(\lambda)|$ is found on the boundary of some region $H$ of the complex plane that includes the spectrum of $A$ and it is sufficient to regard the problem as being defined on the boundary. Smolarski and Saylor [10] suggest the use of the least squares residual polynomial minimizing the $L_2$ norm $\parallel 1 - \lambda s_n(\lambda) \parallel_w$ with respect to some weight $w(\lambda)$ on the boundary of $H$. Suppose that the $\mu + 1$ points $h_0, h_1, \cdots, h_\mu$ constitute the vertices of $H$. On each edge $E_\nu$ of the convex hull, $\nu = 1, \cdots, \mu$, we choose a weight function $w_\nu(\lambda)$. Denoting by $c_\nu$ the center of the $\nu$th edge and by $d_\nu$ the half width, i.e., $c_\nu = \frac{1}{2}(h_\nu + h_{\nu-1}), \qquad d_\nu = \frac{1}{2}(h_\nu - h_{\nu-1})$, the weight function on each edge is defined by $w_\nu(\lambda) = \frac{2}{\pi}|d_\nu^2 - (\lambda - c_\nu)^2|^{-\frac{1}{2}}$. The inner product on the space of complex polynomials is defined by $< p, q >= \sum_{\nu=1}^{\mu} \int_{E_\nu} p(\lambda)\overline{q(\lambda)} w_\nu(\lambda) |d\lambda|$. An algorithm using explicitly the modified moments $< t_i(\lambda), t_j(\lambda) >$, where $\{t_j\}$ is some suitable basis of polynomials, is developed for the problem of computing the least squares polynomials in the complex plane.

We express the polynomial $t_j(\lambda)$ in terms of the Tchebychev polynomials $t_j(\lambda) = \sum_{i=0}^{j} \gamma_{i,j}^{(\nu)} T_i(\xi)$ where $\xi = (\lambda - c_\nu)/d_\nu$ is real. The expansion coefficients $\gamma_{i,j}^{(\nu)}$ can be computed easily from the three term recurrence of the polynomials $\beta_{k+1} t_{k+1}(\lambda) = (\lambda - \alpha_k) t_k(\lambda) - \delta_k t_{k-1}(\lambda)$. The problem $\min_{s \in P_{n-1}} \parallel 1 - \lambda s_n(\lambda) \parallel_w$ is to find $\eta = (\eta_0, \eta_1, \cdots, \eta_{n-1})^T$ of $s_n(\lambda) = \sum_{i=0}^{n-1} \eta_i t_i(\lambda)$ so that $J(\eta) = \parallel 1 - \lambda s_n(\lambda) \parallel_w$ is minimum.

### 2.4 Approach

In the previous section we described the outline of the least-squares based method on any arbitrary area. It has a difficulty on the application to other purposes due to the constraint $P_n(0) = 1$.

We use the fact that the eigenvalue problem does not require any such condition to the polynomial and propose a new simple algorithm to get the mini-max polynomial to accelerate the convergence of the projection method. The minimum property of the Tchebychev functions described below is important to prove the optimality of this polynomial.

Let a non-negative weight function $w(\lambda)$ be given in the interval $a \geq \lambda \geq b$. The orthogonal polynomials $p_0(\lambda), p_1(\lambda), \cdots$, when multiplied by suitable factors $C$, possess a minimum property:

the integral $\int (\lambda^n + a_{n-1}\lambda^{n-1} + \cdots + a_0)^2 w(\lambda) d\lambda$ takes on its least value when the polynomial in the integrand is $C p_n(\lambda)$. The polynomial in the integrand may be written as a linear combination of the $p_i(\lambda)$, in the form $(C p_n(\lambda) + c_{n-1} p_{n-1}(\lambda) + \cdots c_0)$. Since the functions $p_n(\lambda)\sqrt{w(\lambda)}$ are orthogonal, and in fact, orthogonal if the $p_i(\lambda)$ are appropriately defined, the integral is equal to $C^2 + \sum_{\nu=0}^{n-1} c_\nu^2$, which assumes its minimum at $c_0 = c_1 = \cdots = c_{n-1} = 0$.

Using the above property, we describe the new method to generate the coefficients of the orthonormal polynomials in terms of the Tchebychev weight below.

We use the three term recurrence

$$\beta_{n+1} p_{n+1}(\lambda) = (\lambda - \alpha_n) p_n(\lambda) - \beta_n p_{n-1}(\lambda),$$

where $p_i(\lambda)$ satisfies the ortho-normality. Because of

the condition of the use of the Tchebychev polynomial

$$p_n(\lambda) = \sum_{i=0}^{n} \gamma_{i,n}^{(\nu)} T_i[(\lambda - c_\nu)/d_\nu],$$

the constraints

$$< p_0, p_0 >= 2 \sum_{\nu=1}^{\mu} |\gamma_{0,0}^{(\nu)}|^2 = 1$$

$$< p_1, p_1 >= \sum_{\nu=1}^{\mu} [2|\gamma_{0,1}^{(\nu)}|^2 + |\gamma_{1,1}^{(\nu)}|^2] = 1$$

$$< p_0, p_1 >= 2 \sum_{\nu=1}^{\mu} \gamma_{0,0}^{(\nu)} \overline{\gamma}_{1,1}^{(\nu)} = 0$$

must hold.

Moreover each expansion of $p_i(\lambda)$ at any edge must be consistent. The condition $2\sum_{\nu=1}^{\mu} |\gamma_{0,0}^{(\nu)}|^2 = 1$ derives

$$|\gamma_{0,0}^{(\nu)}| = \frac{1}{2\mu}, \qquad \nu = 1, \cdots \mu,$$

and we can choose $\frac{1}{\sqrt{2\mu}}$ as $\gamma_{0,0}^{(\nu)}$. The consistency of

$$p_1(\lambda) = \gamma_{0,1}^{(\nu)} + \gamma_{1,1}^{(\nu)}(\lambda - c_\nu)/d_\nu$$

$$= (\gamma_{1,1}^{(\nu)}/d_\nu)\lambda + \gamma_{0,1}^{(\nu)} - \gamma_{1,1}^{(\nu)} c_\nu/d_\nu$$

derives

$$\gamma_{1,1}^{(\nu)}/d_\nu = \gamma_{1,1}^{(\nu')}/d_{\nu'},$$

$$\gamma_{0,1}^{(\nu)} - \gamma_{1,1}^{(\nu)} c_\nu/d_\nu = \gamma_{0,1}^{(\nu')} - \gamma_{1,1}^{(\nu')} c_{\nu'}/d_{\nu'} \qquad (\nu \neq \nu').$$

It can be rewritten as

$$\gamma_{1,1}^{(\nu)} = d_\nu t, \qquad \gamma_{0,1}^{(\nu)} - c_\nu t = \gamma_{0,1}^{(\nu')} - c_{\nu'} t$$

where $t$ is a real number.

Using the condition

$$< p_0, p_1 >= \sum_{\nu=1}^{\nu} \gamma_{0,0}^{(\mu)} \overline{\gamma_{0,1}^{(\nu)}} = \sum_{\nu=1}^{\mu} \frac{1}{\sqrt{2\mu}} \overline{\gamma_{0,1}^{(\nu)}} = 0,$$

the sum

$$\sum_{\nu=1}^{\mu} (\gamma_{0,1}^{(\nu)} - c_\nu t) = -\sum_{\nu=1}^{\mu} c_\nu t = \mu(\gamma_{0,1}^{(\nu')} - c_{\nu'} t)$$

$$(1 \leq \nu' \leq \mu)$$

derives the relation

$$\gamma_{0,1}^{(\nu)} = c_\nu t - (\sum_{\nu'=1}^{\mu} c_{\nu'})t/\mu.$$

Putting it into the equation

$$< p_1, p_1 >= \sum_{\nu=1}^{\mu} [2|\gamma_{0,1}^{(\nu)}|^2 + |\gamma_{1,1}^{(\nu)}|^2] = 1,$$

we have

$$2\sum_{\nu=1}^{\mu} |c_\nu - (\sum_{\nu'=1}^{\mu} c_{\nu'})/\mu|^2 t^2 + \sum_{\nu=1}^{\mu} |d_\nu|^2 t^2 = 1.$$

It derives $t = 1/\sqrt{S}$ where

$$S = \sum_{\nu=1}^{\mu} [2|c_\nu - (\sum_{\nu'=1}^{\mu} c_{\nu'})/\mu|^2 + |d_\nu|^2].$$

From the above constraints, we can determine the values of all the coefficients of the polynomial using the values of $d_\nu, c_\nu$,and $\mu$.

## 3 Algorithm

We describe the details of our algorithm. We begin with the definition of the notations. The minimax polynomial, which is derived by the definition of the new norm on the boundary, is combined with the Arnoldi method as an accelerator. We mention some points to notice when we use the algorithm.

### 3.1 The definition of the $L_2$ norm

This section defines the $L_2$ norm on the boundary of the convex hull and other notations. We described in the previous section the outline of the method by the least squares polynomials, which is based on the convex hull generated from the unwanted eigenvalues. In this section we begin with the computation of the convex hull.

Suppose a nonsymmetric matrix $A$ is given. We must implement some adaptive scheme in order to estimate the approximate eigenvalues. The combination of the eigensolver and the accelerating technique is described subsequently.

Nonsymmetric matrices have complex eigenvalues which distribute symmetrically in terms of the real axis. Hence we can consider only the upper half of the complex plane. Using the sorted eigenvalues, we start from the rightmost point and make it the vertex $h_0$ of the convex hull $H$. We compute the gradient between $h_i$ and the other eigenvalues with smaller real parts, and choose the point with the smallest gradient as $h_{i+1}$.

Since the eigenvalues obtained by the Arnoldi method is roughly ordered in terms of the absolute value, the adoption of the bubble sort is appropriate. This algorithm uses the property that only the points in the upper half plane are concerned. It requires $O(n^2)$ complexity in the worst case and $O(n)$ in the best case.

We then define the $L_2$ norm on the boundary of the convex hull $H$ constituted by the points $h_0, \cdots, h_\mu$. On each edge $E_\nu \quad (\nu = 1, 2, \cdots \mu)$, we denote the center and the half width by $c_\nu = \frac{1}{2}(h_\nu + h_{\nu-1})$ and $d_\nu = \frac{1}{2}(h_\nu - h_{\nu-1})$, respectively, and define the weight function by

$$w_\nu(\lambda) = \frac{2}{\pi}[d_\nu^2 - (\lambda - c_\nu)^2]^{-\frac{1}{2}} \qquad (\lambda \in E_\nu).$$

Using the above definition, the inner product on $\partial H$ is defined by

$$< p, q >= \int_{\partial H} p(\lambda)\overline{q(\lambda)}w(\lambda)|d\lambda|$$

$$= \sum_{\nu=1}^{\mu} \int_{E_\nu} p(\lambda)\overline{q(\lambda)}w_\nu(\lambda)|d\lambda| = \sum_{\nu=1}^{\mu} < p, q >_\nu .$$

$\| p(\lambda) \|_w =< p, p >^{\frac{1}{2}}$ satisfies the following theorem.

**Theorem 1** *In an inner product space, the norm* $\| u \|$ *of an element* $u$ *of the complex linear space has the following properties:*

1. $\| ku \| = |k| \| u \|$.
2. $\| u \| > 0$ *unless* $u = 0$; $\| u \| = 0$ *implies* $u = 0$.
3. $\| u + v \| \leq \| u \| + \| v \|$.

### 3.2 The computation of the coefficient $\gamma$

We have mentioned the expression of the polynomial i.e.,

$$p_n(\lambda) = \sum_{i=0}^{n} \gamma_{i,n}^{(\nu)} T_i[\frac{\lambda - c_\nu}{d_\nu}].$$

Using the three term recurrence of the Tchebychev polynomials, a similar recurrence

$$\beta_{k+1}p_{k+1}(\lambda) = (\lambda - \alpha_k)p_k(\lambda) - \delta_k p_{k-1}(\lambda)$$

on the $p_i(\lambda)$ holds. Denoting $\xi_\nu$ by $\xi_\nu = (\lambda - c_\nu)/d_\nu$, the equation can be rewritten as

$$\beta_{k+1}p_{k+1}(\lambda)$$

$$= (d_\nu \xi + c_\nu - \alpha_k) \sum_{i=0}^{k} \gamma_{i,k}^{(\nu)} T_i(\xi) - \delta_k \sum_{i=0}^{k-1} \gamma_{i,k-1}^{(\nu)} T_i(\xi).$$

From the relations

$$\xi T_i(\xi) = \frac{1}{2}[T_{i+1}(\xi) + T_{i-1}(\xi)] \quad i > 0, \qquad \xi T_0(\xi) = T_1(\xi),$$

it is expressed by

$$\sum \gamma_i \xi T_i(\xi) = \frac{1}{2}\gamma_1 T_0(\xi) + (\gamma_0 + \frac{1}{2}\gamma_2)T_1(\xi)$$

$$+ \cdots + \frac{1}{2}(\gamma_{i-1} + \gamma_{i+1})T_i(\xi) + \cdots + \frac{1}{2}(\gamma_{n-1} + \gamma_{n+1})T_n(\xi)$$

$$(\gamma_{n+1} = 0).$$

It is arranged into

$$\beta_{n+1}p_{n+1}(\lambda) = d_\nu[\frac{\gamma_{1,n}^{(\nu)}}{2} T_0(\xi) + (\gamma_{0,n}^{(\nu)} + \frac{\gamma_{2,n}^{(\nu)}}{2})T_1(\xi)$$

$$+ \cdots + \sum_{i=2}^{n} \frac{1}{2}(\gamma_{i-1,n}^{(\nu)} + \gamma_{i+1,n}^{(\nu)})T_i(\xi)]$$

$$+ (c_\nu - \alpha_n) \sum_{i=0}^{n} \gamma_{i,n}^{(\nu)} T_i(\xi) - \delta_n \sum_{i=0}^{n-1} \gamma_{i,n-1}^{(\nu)} T_i(\xi)$$

$$(T_{-1} = T_1).$$

Comparing the equation with

$$p_{n+1}(\lambda) = \sum_{i=0}^{n+1} \gamma_{i,n+1}^{(\nu)} T_i(\xi),$$

we find the following relations

$$\beta_{n+1}\gamma_{0,n+1}^{(\nu)} = \frac{1}{2}d_\nu \gamma_{1,n}^{(\nu)} + (c_\nu - \alpha_n)\gamma_{0,n}^{(\nu)} - \delta_n \gamma_{0,n-1}^{(\nu)},$$

$$\beta_{n+1}\gamma_{1,n+1}^{(\nu)} = d_\nu(\gamma_{0,n}^{(\nu)} + \frac{1}{2}\gamma_{2,n}^{(\nu)}) + (c_\nu - \alpha_n)\gamma_{1,n}^{(\nu)} - \delta_n \gamma_{1,n-1}^{(\nu)},$$

and

$$\beta_{n+1}\gamma_{i,n+1}^{(\nu)} = \frac{d_\nu}{2}[\gamma_{i+1,n}^{(\nu)} + \gamma_{i-1,n}^{(\nu)}] + (c_\nu - \alpha_n)\gamma_{i,n}^{(\nu)} - \delta_n \gamma_{i,n-1}^{(\nu)}$$

$$i = 2, ..., n+1 \qquad (\gamma_{-1,n}^{(\nu)} = \gamma_{1,n}^{(\nu)}, \quad \gamma_{i,n}^{(\nu)} = 0 \quad i > n).$$

The choice of the initial values $\gamma_{0,0}^{(\nu)}$, $\gamma_{0,1}^{(\nu)}$ and $\gamma_{1,1}^{(\nu)}$ is described in the previous section.

### 3.3 The computation of the coefficients in the three term recurrence

Using the relation

$$\beta_{k+1}p_{k+1}(\lambda) = (\lambda - \alpha_k)p_k(\lambda) - \delta_k p_{k-1}(\lambda)$$

and the orthogonality of the Tchebychev polynomials, we derive

$$\beta_{k+1} =< p_{k+1}, p_{k+1} >^{1/2}$$

$$= \sum_{\nu=1}^{\mu} \int_{E_\nu} p_{k+1}\overline{p_{k+1}} w_\nu(\lambda)|d\lambda|$$

$$= \sum_{\nu=1}^{\mu} {\sum_{i=0}^{k+1}}' \gamma_{i,k+1}^{(\nu)} \overline{\gamma_{i,k+1}^{(\nu)}}$$

where we denote by $\sum'$

$${\sum_{i=0}^{n}}' a_i = 2a_0 + \sum_{i=1}^{n} a_i.$$

$\alpha$ and $\delta$ are computed similarly:

$$\alpha_k =< \lambda p_k, p_k >$$

$$= \sum_{\nu=1}^{\mu} (c_\nu {\sum_{i=0}^{k}}' \gamma_{i,k}^{(\nu)} \overline{\gamma_{i,k}^{(\nu)}} + d_\nu {\sum_{i=0}^{k}}' \gamma_{i,k}^{(\nu)} \overline{\gamma_{i+1,k}^{(\nu)}}),$$

$$\delta_k =< \lambda p_k, p_{k-1} >= \sum_{\nu=1}^{\mu} d_\nu v_\nu$$

where

$$v_\nu = \gamma_{1,k}^{(\nu)} \overline{\gamma_{0,k-1}^{(\nu)}} + (\gamma_{0,k}^{(\nu)} + \frac{1}{2}\gamma_{2,k}^{(\nu)}) \overline{\gamma_{1,k-1}^{(\nu)}} + \sum_{i=2}^{k-1} \frac{1}{2}(\gamma_{i-1,k}^{(\nu)} + \gamma_{i+1,k}^{(\nu)}) \overline{\gamma_{i,k-1}^{(\nu)}}.$$

### 3.4 The polynomial iteration

The polynomial obtained in the above procedure is applied to the matrix of the problem. We describe the algorithm combined with the Arnoldi method. The Arnoldi method is expressed as follows.

$$\hat{v}_{j+1} = Av_j - \sum_{i=1}^{j} h_{ij} v_i, \quad h_{ij} = (Av_j, v_i), \quad i = 1, ..., j,$$

$$h_{j+1,j} =\| \hat{v}_{j+1} \|, \qquad v_{j+1} = \hat{v}_{j+1}/h_{j+1,j}$$

where $v_1$ is an arbitrary non-zero initial vector. The eigenvectors corresponding to the eigenvalues which have the largest real parts are selected and combined linearly. The remaining eigenvalues constitute the convex hull. Suppose we have each coefficients of the polynomial $p_n(\lambda)$, where $n$ is some appropriate integer. Put the combined vector into $v_0$ and we obtain the new vector $v_n$ in which the components of the necessary eigenvectors are amplified by operating the following recursion:

$$p_0(A)v_0 = \gamma_{0,0}^{(\nu)} Ev_0 \qquad (1 \le \nu \le \mu)$$

$$p_1(A)v_0 = \gamma_{0,1}^{(\nu)} Ev_0 + \gamma_{1,1}^{(\nu)}/d_\nu \cdot (A - c_\nu E)v_0$$

$$p_{i+1}(A)v_0 = [(A - \alpha_i E)p_i(A)v_0 - \delta_i p_{i-1}(A)v_0]/\beta_{i+1}.$$

Denoting $p_i(A)v_0$ by $w_i$, the above recurrence is transformed into

$$w_0 = \gamma_{0,0}^{(\nu)} v_0$$

$$w_1 = \gamma_{0,1}^{(\nu)} v_0 + \gamma_{1,1}^{(\nu)}/d_\nu \cdot (Av_0 - c_\nu v_0)$$

$$= (\gamma_{0,1}^{(\nu)} - \gamma_{1,1}^{(\nu)} c_\nu/d_\nu)v_0 + \gamma_{1,1}^{(\nu)}/d_\nu \cdot Av_0$$

$$w_{i+1} = [Aw_i - \alpha_i w_i - \delta_i w_{i-1}]/\beta_{i+1} \qquad (i = 2, \cdots, n_T).$$

We mention the calculation of the complex eigenvector [11]. Suppose that the components of $x_2, \cdots, x_n$ has been eliminated and we have

$$u_s = \alpha_1 x_1 + \overline{\alpha}_1 \overline{x_1}, \qquad v_{s+1} = Au_s = \alpha_1 \lambda_1 x_1 + \overline{\alpha_1 \lambda_1 x_1}.$$

If we write

$$\alpha_1 x_1 = z_1 + iw_1, \qquad \lambda_1 = \xi_1 + i\eta_1$$

then

$$u_s = 2z_1, \qquad v_{s+1} = 2\xi_1 z_1 - 2\eta_1 w_1,$$

$$z_1 + iw_1 = \frac{1}{2}[u_s + i(\xi_1 u_s - v_{s+1})/\eta_1].$$

Apart from a normalizing factor we have therefore

$$x_1 = \eta_1 u_s + i(\xi_1 u_s - v_{s+1}).$$

## 4 The complexity

### 4.1 The orthogonality-based method

We use the number of multiplications as the measure of complexity. The QR method requires $4n^2$ multiplications in one complete step, where we denote by $n$ the order of the matrix. The double-shifted QR method, which we use for our problem, requires $8n^2$ multiplications in one step in which the two shifts concerning a conjugate pair are performed [11]. Hence, denoting the number of the steps of the QR method by $n_{QR}$, we see that $4n^2 n_{QR}$ real multiplications are necessary to solve the eigenvalue problem of the matrix $A$.

The complexity of the Arnoldi method with the reorthogonalization, which uses the QR method to compute the eigenvalues of the Hessenberg matrix, is estimated using the above result. It follows the algorithm of the orthogonality-based method.

We require in the $r$th step of the computation of $h_{ir}, \quad i = 1, \cdots, r+1$, $n^2 + 2nr + 2nr + n$ real multiplications. The total complexity required to obtain the Hessenberg matrix $H$ of order $m_A$ is, therefore,

$$m_A n^2 + 2m_A(m_A+1)n + (m_A - 1)n$$

$$= m_A n^2 + (2m_A^2 + 3m_A - 1)n$$

real multiplications. Adding this to the computation of the eigenvalues of $H$ by the QR method, the complexity of the Arnoldi method is approximately given by $m_A n^2 + (2m_A^2 + 3m_A - 1)n + 4m_A^2 n_{QR}$ real multiplications.

The evaluation of the complexity of the orthogonality based method is as follows:

1. The computation of the eigenvalue estimates requires

   $$m_A n^2 + (2m_A^2 + 3m_A - 1)n + 4m_A^2 n_{QR}$$

   real multiplications.

2. Suppose that we have $\mu$ vertices for the convex hull. The computation of the coefficients $\gamma_{i,j}^{(\nu)}$ requires

   $$\mu(6 + \sum_{n=1}^{n_T}(3+4+3n)) \approx \mu[\frac{3}{2}(n_T)^2 + \frac{17}{2}n_T]$$

   complex multiplications where $n_T$ is the order of the polynomial. Each complexity of the other coefficients i.e., $\beta$, $\alpha$, and $\delta$, is

   $$\mu \sum_{i=2}^{n_T}(i+1) \approx \mu[(n_T)^2 + 3n_T],$$

   $$\mu \sum_{i=1}^{n_T-1}[(i+1)+(i+1)] \approx \mu[2(n_T)^2 + 6n_T],$$

   and

   $$\mu\{\sum_{i=1}^{n_T-1}[1+1+2+2(i-2)]\} = \mu[2(n_T)^2 - 2n_T]$$

   complex multiplications, respectively. The total number of the complex multiplications is approximately $\frac{1}{2}\mu[13(n_T)^2 + 31n_T]$.

3. The polynomial iteration requires

   $$n+1+n+n^2+(n_T-1)(n^2+n+n) \approx n_T n^2 + 2n_T n$$

   complex multiplications.

The total computation of the orthogonality-based method for an iteration consists of the sum of those of the three parts, i.e.,

$$m_A n^2 + (2m_A^2 + 3m_A - 1)n + 4m_A^2 n_{QR}$$

real multiplications and

$$n_T n^2 + 2n_T n + \frac{1}{2}\mu[13(n_T)^2 + 31n_T]$$

complex multiplications.

### 4.2 The additional cost of the least-squares based method

The complexity of the least-squares based method is larger, since we need the additional computation of the least squares polynomial using the mini-max polynomials of degree $i = 0, \cdots, n$, which are obtained by our method, as an ortho-normal basis.

The total superfluous cost of the computation of the least squares polynomial is $\frac{1}{6}(n+1)(n+2)(n+3)$ complex multiplications and $\frac{1}{6}n(n+1)(2n+1)$ real multiplications.

### 4.3 The complexity of the Manteuffel's method

The complexity of the computation of the best ellipse [4] is rather complicated. It depends on the distribution of the eigenvalues obtained by the Arnoldi method and classified into several cases.

1. When a pair-wise best point is the mini-max solution, the required computation per a pair of eigenvalues is at most 7 real multiplications and the solution of a cubic equation, if the imaginary parts of the two points are equal. If they are not, 78 real multiplications and the solution of the equation of the fifth degree are required. Moreover we need the judgment whether the other eigenvalues are in the ellipse or not. The number of pairs is $\frac{1}{2}m_A(m_A-1)$ where we denote by $m_A$ the number of the eigenvalues.

2. If no pair-wise best point is the solution, we need the computation of the candidate ellipse for every combination of three points, which contains 48 real multiplications for $\frac{1}{6}m_A(m_A-1)(m_A-2)$ combinations. Then the ellipse with the smallest convergence factor must be chosen.

The complexity of the Newton's method for the nonlinear equations depends on the initial value. Considering that it is used for every combination of the

eigenvalues, we can conclude that the orthogonality-based method, whose complexity of the corresponding part is $\frac{1}{2}\mu[13(n_T)^2 + 31n_T]$ is better.

### 4.4 Other arguments

The speed of linear convergence of the QR method is controlled by $\max_{r=1,\cdots,n-1} |\lambda_{r+1}/\lambda_r|$. With shifts of origin, the convergence of $a_{nn}^{(k)}$ to an eigenvalue is asymptotically quadratic.

The study of the convergence of the Arnoldi method is far less sufficient than that of the Lanczos method, since the theory of the uniform approximation on a compact set in the complex plane is not so advanced [2].

## 5 Numerical Experiments

This chapter reports the results of the numerical experiments of our new method and evaluates its performance. The experiments are performed on a HP9000/720, using double precision.

We start from the decision of each element of the matrix given in the problem. In this section, the scaled sequences of random numbers are assigned respectively to the real and the imaginary parts of the eigenvalues except for those which are to be selected. The matrices are block diagonals with $2 \times 2$ or $1 \times 1$ diagonal blocks. Each block is of the form

$$\begin{bmatrix} a & b/2 \\ -2b & a \end{bmatrix}$$

to prevent the matrix to be normal and has eigenvalues $a \pm bi$. It is transformed by an orthogonal matrix generated from a matrix with random elements by the Schmidt's orthogonalization method. $m_A$ and $n_T$ denote the order of the Arnoldi method and the maximum order of the Tchebychev polynomials respectively. We compare this algorithm with the double-shifted QR method [12].

In the orthogonality-based method, the $\lambda_{\max}$ is computed by $\tilde{\lambda} = \| \tilde{x}_{i+1} \|_2 / \| \tilde{x}_i \|_2$ where $\tilde{x}_{i+1} = A\tilde{x}_i$, since we suppose that the maximum eigenvalue is a positive real number.

The error is computed by the $L_2$ norm. The computation time is measured by HP9000/720, where the unit is $\frac{1}{60}$ second.

The complexity of the orthogonality-based method can be seen to be roughly $O(n^2)$ as our evaluation which we made in the previous chapter indicates, while that of the QR method $O(n^3)$.

The relation between the error and the parameters of the orthogonality-based method is given in Figure 1. We denote the degree of the polynomial by $n$ and the order of the Arnoldi method by $m$. This graph shows that the order of the Arnoldi method has the closer correlation with the error than the degree of the orthogonality-based method. This is caused by the fact that the Arnoldi method can not always obtain the eigenvalue of the largest modulus.

We adopt the iterative Arnoldi method in the orthogonality-based method. The Arnoldi method performed for reference is also made iterative.

In this section we test the five variations of the distribution of the eigenvalues using the matrices of order 50. The cases of $\lambda_{\max} = 2, 1.5$, and 1.1 while the distribution of the other eigenvalues is $\Re\lambda \in [0,1]$, and $\Im\lambda \in [-1,1]$. We denote the number of the iterations by $i_A$.

**Case 1**

$\lambda_{\max}$ is 2, while the distribution of the other eigenvalues is $\Re\lambda \in [0,1]$, $\Im\lambda \in [-1,1]$. The effect of the iteration is significant, especially for the orthogonality-based method. This tendency becomes sharper as the maximum eigenvalue gets closer to the second eigenvalue.

**Case 2**

The maximum eigenvalue is 1.5, while the distribution of the other eigenvalues is $\Re\lambda \in [0,1]$, $\Im\lambda \in [-1,1]$. Some variations of the combination of the parameters $i_A$ and $n_T$ are examined. The best combination of the parameters is not trivial and the consideration on this problem is given in the last section.

**Case 3**

The maximum eigenvalue is 1.1, while the distribution of the other eigenvalues is: $\Re\lambda \in [0,1]$, $\Im\lambda \in [-1,1]$. In this test we examine the relation between the parameter $i_A$ and the order of the Arnoldi method $m_A$. The table shows that it is more effective to decrease the order of the Arnoldi method than to decrease the number of the Arnoldi iteration.

## 6 Conclusion

We proposed the iterative Arnoldi method using the orthogonality of the Tchebychev polynomials for the large nonsymmetric eigenvalue problem.

This method requires the computation of $m_A n^2 + (2m_A^2 + 3m_A - 1)n + 4m_A^2 n_{QR}$ real multiplications and $n_T n^2 + 2n_T n + \frac{1}{2}\mu\{13(n_T)^2 + 31n_T\}$ complex multiplications, which is less than those of the method by the Manteuffel's optimal ellipse technique, which requires the solutions of nonlinear equations and $O(n^3)$ computations for every combination of eigenvalues in most cases, and the least squares method, which costs $O(n^3)$ superfluous complexity.

We examined the other problems such as computational error by numerical experiments. Our algorithm shows the best performance in most conditions except for the case where the moduli of some unwanted close eigenvalues is much larger than those of the necessary eigenvalues. In such a case we can not obtain the wanted eigenvalues. The deflation seems to be the most hopeful technique to get rid of them and continue the process. We need some additional study for this difficulty.

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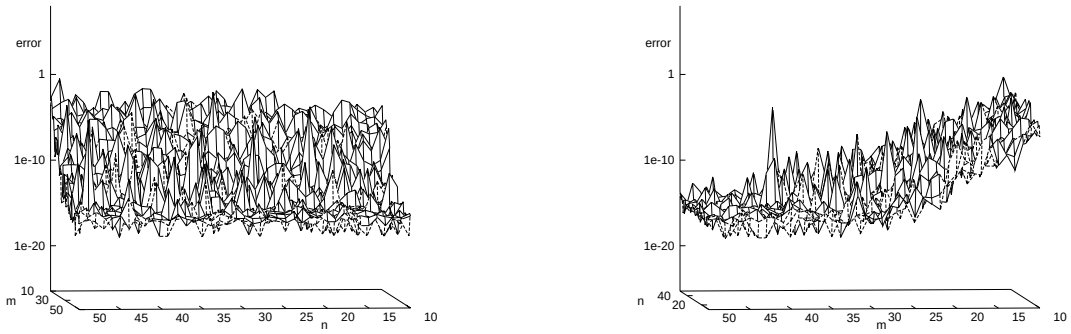


Figure 1: The relation between the error and the parameters $n$, $m$ of the orthogonality-based method

| orthogonality-based | | | | | Arnoldi | | | | QR | |
|---|---|---|---|---|---|---|---|---|---|---|
| $i_A$ | $m_A$ | $n_T$ | error | time | $i_A$ | $m_A$ | error | time | error | time |
| 1 | 5 | 15 | 1.1E-10 | 11 | 1 | 15 | 2.3E-09 | 18 | 5.1E-15 | 112 |
| 2 | 5 | 15 | 3.6E-15 | 23 | 2 | 15 | 8.9E-16 | 34 | | |

Table 1: $\lambda_{\max} = 2$, the distribution of the other eigenvalues : $\Re\lambda \in [0,1]$, $\Im\lambda \in [-1,1]$

| orthogonality-based | | | | | Arnoldi | | | | QR | |
|---|---|---|---|---|---|---|---|---|---|---|
| $i_A$ | $m_A$ | $n_T$ | error | time | $i_A$ | $m_A$ | error | time | error | time |
| 1 | 5 | 15 | 5.0E-05 | 15 | 1 | 15 | 1.2E-05 | 17 | 3.6E-15 | 111 |
| 2 | 5 | 15 | 1.1E-08 | 25 | 2 | 15 | 5.3E-11 | 33 | | |
| 3 | 5 | 15 | 1.9E-11 | 32 | 3 | 15 | 3.7E-15 | 49 | | |
| 4 | 5 | 15 | 5.6E-14 | 42 | 4 | 15 | 3.3E-15 | 63 | | |
| 5 | 5 | 15 | 3.4E-15 | 54 | 5 | 15 | 2.8E-15 | 79 | | |
| 3 | 5 | 20 | 3.0E-15 | 42 | 3 | 15 | 3.7E-15 | 49 | | |
| 3 | 5 | 19 | 8.9E-16 | 38 | | | | | | |
| 3 | 5 | 18 | 4.5E-13 | 38 | | | | | | |
| 1 | 5 | 60 | 1.3E-14 | 47 | | | | | | |

Table 2: $\lambda_{\max} = 1.5$, the distribution of the other eigenvalues : $\Re\lambda \in [0,1]$, $\Im\lambda \in [-1,1]$

| orthogonality-based | | | | | Arnoldi | | | | QR | |
|---|---|---|---|---|---|---|---|---|---|---|
| $i_A$ | $m_A$ | $n_T$ | error | time | $i_A$ | $m_A$ | error | time | error | time |
| 1 | 50 | 10 | 3.2E-15 | 240 | 1 | 50 | 7.5E-13 | 235 | 5.2E-15 | 113 |
| 1 | 45 | 20 | 6.9E-15 | 206 | 1 | 45 | 4.1E-10 | 191 | | |
| 2 | 30 | 20 | 3.2E-15 | 161 | 2 | 50 | 7.7E+00 | 531 | | |
| 3 | 20 | 15 | 6.3E-12 | 111 | 1 | 50 | 7.5E-13 | 236 | | |
| 4 | 15 | 20 | 3.5E-13 | 112 | | | | | | |
| 5 | 10 | 20 | 2.9E-14 | 96 | | | | | | |

Table 3: $\lambda_{\max} = 1.1$, the distribution of the other eigenvalues : $\Re\lambda \in [0,1]$, $\Im\lambda \in [-1,1]$