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How to Compute the Smallest / Largest Eigenvalue of a Symmetric Matrix

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Abstract

In this paper we develop a general Homotopy method called the Group Homotopy method to solve the symmetric eigenproblem. The Group Homotopy method overcomes notable drawbacks of the existing Homotopy method, namely, (i) the possibility of breakdown or having a slow rate of convergence in the presence of clustering of the eigenvalues and (ii) the absence of any definite criterion to choose a step size that guarantees the convergence of the method. On the other hand, We also have a good approximations of the largest eigenvalue of a Symmetric matrix from Lanczos algorithm. We apply it for the largest eigenproblem of a very large symmetric matrix with a good initial points.

1 Introduction

We have developed a general Homotopy method for the eigenvalue problem of a Symmetric matrix. A general Homotopy method called, the group Homotopy method has attractive features that it preserves the structure of the original matrix and finds a specific eigenvalue without computing any other eigenvalues, in contract with the existing methods which destroy the structure during similarity transformation. Since the method preserves the special structure of matrices, it is quite suitable to obtain eigenpairs of a class of matrices which possesses some special characteristics that we might take advantage. In this paper, we present the method how to find extreme eigenvalues of a Symmetric matrix. Recall that a Homotopy method for the eigenvalue problem is in the following. Let $A \in M_n$ be Symmetric. Then there is a orthogonal

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$U = [U_1 \ \dots \ U_n] \in M_n$ such that $A = U \begin{bmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{bmatrix} U^T$ where $\lambda_k \in R$ are the eigenvalues and $U_k \in R^n$ are the corresponding eigenvectors of A for k=1,...,n. We denote by $\begin{bmatrix} u_k \\ \lambda_k \end{bmatrix} \in R^n \times R$ the eigenpair of A for k=1,...,n. Note that since $\{U_k\}_{k=1,\dots,n}$ is linearly independent $\left\{ \begin{bmatrix} U_k \\ \lambda_k \end{bmatrix} \right\}$ is linearly independent. We denote by σ(A) the set of eigenvalues of A(including multiplicities). Suppose the eigenvalue $\lambda_k \in \sigma$(A) has the algebraic multiplicity p, i.e., $\lambda_k = \lambda_{k+1} = \cdots = \lambda_{k+p}$. Then we note that any $X \in$ span $\{U_i\}_{i=k,\cdots,k+p}$is an eigenvector for λ_k. Thus an eigenpair $\begin{bmatrix} U_k \\ \lambda_k \end{bmatrix}$ is not unique. Let $S \in M_n$ be the initial Symmetric matrix with eigenpairs $\begin{bmatrix} X_k \\ \alpha_k \end{bmatrix}$ for k=1,...,n that are known. Let $A \in M_n$ be the objective Symmetric matrix with eigenpairs $\begin{bmatrix} U_k \\ \lambda_k \end{bmatrix}$ for k=1,...,n are to be obtained. Define a mapping $H : \mathbb{R} \longrightarrow M_n$ such that

$$H(t) = A(t) \equiv (1-t)S + tA, \quad t \in [0,1].$$

Note that $A(t) = S + t(A - S)$ so that the matrix $A(t)$ can be made close to S by choosing t small enough. The objective is to obtain the set of all the eigenpairs $\left\{ \begin{bmatrix} U_k \\ \lambda_k \end{bmatrix} \right\}$, $k = 1, \dots, n$ of $A(1) = A$ by successively obtaining the set of eigenpairs $\left\{ \begin{bmatrix} U_k^{(i)} \\ \lambda_k^{(i)} \end{bmatrix} \right\}, k = 1, \dots, n$ of $A(t_i), 0 = t_0 < t_1 < \cdots < t_n = 1$, starting from the set of eigenpairs $\left\{ \begin{bmatrix} x_k \\ \alpha_k \end{bmatrix} \right\}, k = 1, \dots, n$ of $A(0) = S$. The procedure is called the Homotopy method [1,4]. From the existing homotopy method, it didn't give us any criterion of the step size Δt . To overcome the absence of any definite criterion to choose a step size that guarantees the convergence of the method, a new Homotopy method called, the individual Homotopy method, is developed [3]. The homotopy method proceeds as following :

Set $t_0 = 0$.

(i) Find t_1, $(t_1 > t_0)$ such that the initial points $\left\{ \begin{bmatrix} x_k(t_0) \\ \alpha_k(t_0) \end{bmatrix} \right\}$ converge to $\left\{ \begin{bmatrix} x_k(t_1) \\ \alpha_k(t_1) \end{bmatrix} \right\}$, for k=1, ...,n under the Newton iteration [1,5,6].

(ii) Obtain $A(t_1) = S + t_1(A - S) = X(t_1)\begin{bmatrix} \lambda_1(t_1) & & 0 \\ & \ddots & \\ 0 & & \lambda_n(t_1) \end{bmatrix} X^T(t_1)$, where $X(t_1) = [X_1(t_1) \cdots X_n(t_1)] \in M_n$ is an orthogonal matrix. Notice that $A(t) = S + t(A - S) = S + t_1(A - S) + (t - t_1)(A - S) = A(t_1) + (t - t_1)(A - S)$ for some $t \in [0,1]$. Hence A(t) can be again made close to $A(t_1)$by choosing some small $t > t_1$. Thus we find $t_2 > t_1$that satisfies the condition (i). In this way, we successively produce that approaches to 1 while obtaining the eigenpairs $\left\{ \begin{bmatrix} x_k(t_1) \\ \alpha_k(t_1) \end{bmatrix} \right\}$ of $A(t_i)$ by the Newton iteration[1,5,6]. We describe the method to compute extreme eigenvalues of a matrix based on the group homotopy.

It is clear that if we can choose an initial matrix properly, then we can reduce the number of iterations. In section 2, we present the group homotopy method with the choice of the initial matrix where the objective matrix is a symmetric matrix. In section 3, 4, we present the applications of computing extreme eigen values and the experiments for the algorithm.

2 Methodology for The Group Homotopy

In the group Homotopy, the choice of an initial matrix can be arbitrary even though a good choice of the initial matrix might facilitate convergence. The group Homotopy is a general Homotopy method in the following senses: (i) Unlike in the existing Homotopy method[1], it gives a definite criterion of how to choose a step size that will guarantee the convergence in the modified Newton Iteration[3]. (ii) The method works regardless of the choice of the initial matrix. (iii) The method guarantees a big enough step size Δt_i so that the group Homotopy method terminates in a finite number of steps and gives all the eigenpairs of the objective matrix. To obtain a group Homotopy method that will accomplish all the above objectives, we carefully examine difficulties that arise in the individual Homotopy[3] method. Assume that an arbitrary Symmetric matrix is chosen as the initial matrix. As we have observed previously, the individual Homotopy method fails whenever the gap between some adjacent eigenvalues of the matrix $A(t)$ becomes quite small. It will occur when some eigenvalues of $A(t)$ are clustered, i. e., there are groups of a consecutive eigenvalues in which the distance between any two groups is much larger than the gaps among the eigenvalues that belong to the same group. We resolve the difficulty by using a concept, called the **group gap**. For that purpose, we define a clustering of eigenvalues as follows:

Definition 2.1 : We say that two adjacent eigenvalues λ_k and λ_{k+1} are clustered if

$|\lambda_k - \lambda_{k+1}| < Gap^*, 1 \geq k \geq k-1$ where is a given positive number.

Definition 2.2 :We say that a subset $G = \{\lambda_k, \lambda_{k+1}, \ldots, \lambda_{k+m}\} \subseteq \sigma(A)$ is a group of clustering of eigenvalues if $|\lambda_{k+i} - \lambda_{k+i+1}| < Gap^*$ for all $i = 0, \ldots, m-1$ where $|\lambda_{k-1} - \lambda_k| \geq Gap^*$ and $|\lambda_{k+m} - \lambda_{k+m+1}| \geq Gap^*$.

From the definition we note the following: Suppose G_1 and G_2 are two distinct groups of clustering eigenvalues in σ(A), $G_1 = \lambda_{1_1}, \cdots, \lambda_{i_s}$and $G_2 = \lambda_{1_1}, \cdots, \lambda_{i_t}$ Then $|\lambda_{i_k} - \lambda_{i_m}| \geq Gap^*$ for all $k = 0, \ldots, s$ and $m = 0, \ldots, t$ Thus, there is a gap, i. e., Gap^* between G_1 and G_2. Note that for the $\Delta t_i = \dfrac{gap^*}{||A-S||_2}$, $gap^* \equiv gap^*(A(t_i))$ individual Homotopy[4]. Now we will make a suitable choice of Gap^* in order to have a big enough step size $\Delta t_i = \dfrac{gap^*}{||A-S||_2}$ for the group Homotopy to ensure the method terminates in a finite steps. We will use the following choice Gap^* of for an actual implementation of the algorithm: (i) $Gap^* = \delta||A-S||_2$ for a suitable $\delta > 0$ or (ii) $Gap^* = \dfrac{\alpha_{max} - \alpha_{min}}{Kn}, K > 0$ a fixed constant where n is the size of the matrix. Now we pay attention to some difficulties that might occur with the group Homotopy by using a group gap. Two serious problems occur with the procedure in this group Homotopy, which requires some detailed discussion to clarity the point. First, in contrast with the individual Homotopy, the Newton iteration may not converge at all under the group Homotopy where the step size $\Delta t_i > 0$ is determined by the group gap, Gap^*. Note that in the individual Homotopy, we give the criterion of the stepsize for Homotopy method.

Theorem 2.3 : Let symmetric matrices A and S be such that

$$A = U \begin{bmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{bmatrix} U^T$$

and

$$S = X \begin{bmatrix} \alpha_1 & & 0 \\ & \ddots & \\ 0 & & \alpha_n \end{bmatrix} X^T,$$

$\lambda_1 \geq \ldots \geq \lambda_n$ and $\alpha_1 \geq \alpha_2 \geq \ldots \geq \alpha_n, U = [U_1 \cdots U_n] \in M_n$ and $X = [X_1 \cdots X_n] \in M_n$ are orthogonal matrices. Then $\begin{bmatrix} X_k \\ \alpha_k \end{bmatrix}$ converges to $\begin{bmatrix} U_k \\ \lambda_k \end{bmatrix}$ for $k = 1, \ldots, n$, under the Newton iteration whenever $||S-A||_2 \leq \dfrac{gap^*(S)}{q}, q \geq 4$.

proof: [3]

Theorem 2.3 ensures if it is chosen such a way that where then the Newton itera-

tion starting with each eigenpair $\begin{bmatrix} X_k(t_i) \\ \alpha_k(t_i) \end{bmatrix}$ of the matrix $A(t_i) = (1-t_i)S + t_iA$ is guaranteed to converge to the corresponding eigenpair $\begin{bmatrix} X_k(t_{i+1}) \\ \alpha_k(t_{i+1}) \end{bmatrix}$ of the matrix $A(t_{i+1}) = (1-t_{i+1})S + t_iA$. But once the clustered eigenvalues are grouped together to produce big enough step size $\Delta t_i = \dfrac{gap^*}{q\|A-S\|_2}$ Theorem 2.3 does not hold and we lose that theoretical guarantee of the convergence with the Newton iteration. We provide an example to illustrate the point.

Example 2.1: Suppose that

$$S = A(0) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -100 \end{bmatrix} \text{ and } A = A(1) = U \begin{bmatrix} 2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -101 \end{bmatrix} U^T$$

where

$$U^T = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

Then

$$\|S-A\|_2 = \left\| \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \right\|_2 = 1.$$

If we choose $Gap^* = |1-(-100)| = 101$ and $q = 4$, then $\dfrac{Gap^*}{q\|A-S\|_2} = \dfrac{101}{4} > 1$. Note the example is constructed such that the eigenvalue 1 (algebraic multiplicity 2) consists a group G of clustered eigenvalues of $S = A(0)$ and the eigenvalues 2 and 0 form the counterpart group G' in the $\sigma(A) = \sigma(A(1))$. Furthermore, the first two components of the vector $Ux_1 = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{bmatrix}$ that corresponds to the group of clustered eigenvalues 1 of S have all the possible weight. Now if we proceed with the Newton iteration (2.4) with $\alpha_1 = 1, x_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$ to obtain the eigenpair of A,

$$\alpha_1^{(1)} = \alpha_1^{(0)} - \frac{1}{\beta^{(0)}} = \alpha_1^{(0)} - \frac{1}{x_1^T(\alpha_1^{(0)}I - A)^{-1}x_1} = -\infty$$

because

$$x_1^T(\alpha_1^{(0)}I - A)^{-1}x_1 = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \end{pmatrix} \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1/102 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{bmatrix} = 0.$$

We resolve the problem by developing a modified Newton method that has a global convergence property. We describe the method in detail in the next section. Now, we discuss one other major difficulty that arises with the group Homotopy. Assume that the convergence of iteration is guaranteed under the modified Newton method. It should be noted that the Homotopy method produces successively a better approximation of the target matrix A as, $t \to 1$ i.e., we obtain the matrix $A(t_{i+1}) = (1 - t_{i+1})S + t_{i+1}A$ from the matrix $A(t_{i+1}) = (1 - t_i)S + t_iA, 0 \leq t < 1$ by the Newton iteration and we conclude that $A(t_{i+1})$ is a better approximation than $A(t_i)$ to the target matrix A. Therefore, the method requires a complete set of eigenpairs at each step of Homotopy to proceed to the next step. Notice that the previous individual Homotopy method automatically gives the complete set of eigenpairs in each step of Homotopy. Suppose $\left\{ \begin{bmatrix} X_k(t_i) \\ \alpha_k(t_i) \end{bmatrix}, \begin{bmatrix} X_{k+1}(t_i) \\ \alpha_{k+1}(t_i) \end{bmatrix}, \begin{bmatrix} X_{k+m}(t_i) \\ \alpha_{k+m}(t_i) \end{bmatrix} \right\}, 1 < m < n$ for some $1 \leq k \leq n$, $k+m \leq n$ is the subset of clustered eigenpairs of $A(t_i)$) that is grouped together, $0 \leq t_i \leq 1$ and let $\Delta t_i > 0$ be obtained from Gap^* under the group gap criterion.

3 Its Applications for Solving the Extreme Eigenvalue Problem

In this section, we consider a definite criterion of the stepsize under the group homotopy method for the eigenproblem of a symmetric matrix. Suppose Δt_i is determined via Gap^* i. e., $\Delta t_i = t_{i+1} - t_i = \dfrac{Gap^*}{q||A - S||_2}$, to obtain all eigenpairs of $A(t_{i+1})$ from $A(t_i)$. It is given that the clustered eigenvalues of $A(t_i)$ are grouped together whenever the gap between two adjacent eigenvalues is less than Gap^*. We show that there are some strong connections between eigenvalues of $A(t_i)$ and $A(t_{i+1})$ under the assumption $||A - S||_2 \leq \dfrac{Gap^*}{q}$. Suppose $\sigma(A(t_i)) = \{\alpha_1 \cdots \alpha_n\}, \alpha_1 \geq \cdots \geq \alpha_n$ is grouped together under the clustering criterion determined by Gap^*, $\sigma(A(t_i)) = \cup_{k=1}^{g} G_k, G_k = \{\alpha_{k_1} \geq \cdots \geq \alpha_{k_s}\}$ is a group of clustering eigenvalues of $A(t_i), s_1 + s_2 + \cdots + s_g = n$. We devide $\sigma(A(t_{i+1})) = \{\lambda_1 \cdots \lambda_n\}, \lambda_1 \geq \cdots \geq \lambda_n$ to form the groups correspond to the grouping in $\sigma(A(t_i))$ such that $\sigma(A(t_i)) = \cup_{k=1}^{g} G_k', G_k' = \{\lambda_{k_1} \geq \cdots \geq \lambda_{k_s}\}, s_1 + s_2 + \cdots + s_g = n$.

We call G'_k the counterpart of G_k. Suppose $||A-S||_2 \leq \frac{Gap^*}{q}$. Then we claim that the counterpart G' is close to G for a large enough q,

Lemma 3.1: Suppose $A, S \in M_n$ are symmetric and let $\lambda_1 \geq \cdots \geq \lambda_n$ and $\alpha_1 \geq \cdots \geq \alpha_n$ be the eigenvalues of A and S respectively. Then $||A-S||_2 = \rho(A-S) \geq max_k\{|\lambda_k - \alpha_k(A-S)|\}$ where $\rho(A-S) = max_k\{|\lambda_k(A-S)/\lambda_k(A-S)$ are the eigenvalues of $(A-S)\}$. Consequently, if $||A-S||_2 \leq \frac{Gap^*}{q}$, then $|\lambda_k - \alpha_k| \leq \frac{Gap^*}{q}$ for all $k = 1, \cdots, n$. Now we make the following observation. Note that $||A(t_{i+1}) - A(t_i)||_2 = |t_{i+1} - t_i|||A-S||_2 = \Delta t_i||A-S||_2 \leq \frac{Gap^*}{q||A-S||_2} \cdot ||A-S||_2 = \frac{Gap^*}{q}$.

Thus, $max_k\{|\lambda_k - \alpha_k|\} \leq \frac{Gap^*}{q}$ by Lemma 3.1, where λ_k and α_k are the eigenvalues of $A(t_{i+1})$and $A(t_i)$, respectively. Therefore, the k-th eigenvalue of $A(t_{i+1})$ must be within $\frac{Gap^*}{q}$ distance from the k-th eigenvalue of $A(t_i)$ for all $k = 1, \cdots, n$. Now we verify the claim statement.

Lemma 3.2: Suppose $||A-S||_2 = \frac{Gap^*}{q}$, $q > 1$ and let G_1 and G_2 be two distinct groups of clustering eigenvalues of $A(t_i)$. If G'_1 and G'_2 are the groups of eigenvalues of $A(t_{i+1})$ counterpart to G_1 and G_2 respectively, then $dist(G'_1, G'_2) \geq (1 - \frac{2}{q})Gap^*$, where $dist(G'_1, G'_2) = min\{|\lambda_s - \lambda_t| / \lambda_s \in G'_1$ and $\lambda_t \in G'_2\}$.

Proof: Suppose G_1 and G_2 are two distinct groups in $A(t_i)$. Then $|\alpha_s - \alpha_t| > Gap^*$ for all $\lambda_s \in G_1$ and $\lambda_t \in G_2$. Now for $\alpha_s \in G'_1$ and $\alpha_t \in G'_2, Gap^* < |\alpha_s - \alpha_t| = |\alpha_s - \lambda_s + \lambda_s - \lambda_t + \lambda_t - \alpha_t| \leq |\alpha_s - \lambda_s| + |\alpha_t - \lambda_t| + |\lambda_s - \lambda_t|$. Since $|\alpha_s - \alpha_s| < \frac{Gap^*}{q}$ and $|\alpha_t - \alpha_t| < \frac{Gap^*}{q}$ by Lemma 3.1, $Gap^* < \frac{2Gap^*}{q} + |\lambda_s - \lambda_t|$, or $|\lambda_s - \lambda_t| > (1 - \frac{2}{q})Gap^*$. Therefore Lemma 3.2 verifies that for a large enough q > 1, any two distinct groups G'_1 and G'_2 are separated by at least $(1 - \frac{2}{q})Gap^*$ distance. Now we verify that the above is enough to guarantee the convergence of α to some $\lambda \in G'$.

Theorem 3.3: Suppose $||A-S||_2 = \frac{Gap^*}{q}$, $q > 1$ and let $G = \{\alpha_{i_1}, \cdots, \alpha_{i_s}\}$ be a group of clustering eigenvalues, $\alpha_{i_s} \leq \cdots \leq \alpha_{i_l}$.

Let $B = \left[\alpha_{i_s} - \frac{Gap^*}{q}, \alpha_{i_1} + \frac{Gap^*}{q}\right] \subseteq R$ be a closed interval. Then the iteration $\{\alpha^{(i)}\}$ under the modified Newton method starting at $\alpha^{(0)} = \alpha \in B$ remain in B, i. e., for all i[5]. Since the modified Newton method is guaranteed to converge, Theorem 3.3 asserts that each $\alpha \in G$ must converge to some eigenvalue $\lambda \in G'$ of $A(t_{i+1})$. We have discussed about the basic idea of the group homotopy in the section 2. Now we want to apply the group homotopy method for computing the extreme eigenvalues

of a Symmetric matrix. First, it is reminded that we can reduce the number of the iterations, if we choose a proper initial matrix. We consider the choice of the initial matrix of the given symmetric matrix. The choice of an initial matrix S is based on how close are located the eigenvalues of the objective matrix A or $||A - S||_2$ is small as possible. In our extreme eigenvalue problem, we use the Lanczos algorithm to choose an initial matrix, tridiagonal matrix(from Lanczos method). The initial matrix provides very good approximations to the extreme eigenvalues of the objective Symmetric matrix. We describe how to choose an initial matrix and the definite stepsize Δt. Given n by n symmetric matrix A and a unit vector v_1, the Lanczos algorithm constructs simultaneously a symmetric tridiagonal matrix T and an orthonormal matrix V such that $T = V^T AV$. We can choose an initial matrix for the extremal eigen problem since some diagonal entries of tridiagonal matrices are close to the extreme eigenvalues of a objective matrix. Suppose $||T - A||_2 = \epsilon$ and $\Delta t_i \equiv t_{i+1} - t_i$. Then note that $||A(t_i - A(t_{i+1})||_2 = ||T + t_i(A - T) - (A + t_{i+1}(A - T))||_2 = ||\Delta t_i(A - T)||_2 = \Delta_i \cdot \epsilon \leq \frac{Gap^*}{q||A-T||_2} \cdot ||A - T||_2 = \frac{Gap^*}{q}$.

4 Algorithm

In this section, we describe two algorithms for simultaneously finding the eigenpairs of an $n \times n$ symmetric matrix A.

4.1 Algorithm I : Modified Newton Iteration with proper initial points

Let $A = (a_{ij}) \in M_n$ be a given symmetric matrix with eigenpairs for k= 1,...,n. Choose S = diag$(\alpha_1^{(0)}, \cdots, \alpha_n^{(0)})$ be to the initial matrix where the diagonal elements of T are arranged in decreasing order.

Step 1: Apply the Lanczos algorithm to get the initial matrix T = $V^T AV$ such that

$$T = \begin{bmatrix} \alpha_1 & \beta_1 & \cdots & 0 \\ \beta_1 & \alpha_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \beta_n - 1 \\ 0 & \cdots & \beta_n - 1 & \alpha_n \end{bmatrix}.$$

(i) Set $v_0 = 0$, $\beta_0 = 1$, $r_0 = v_1$.

(ii) $v_j = \frac{r_{j-1}}{\beta_{j-1}}$, $\alpha_j = v_j^T A v_j$, $r_j = (A - \alpha_j I)v_j - \beta_{j-1}v_{j-1}$.

(iii) $\beta_j = ||r_j||_2$.

Step 2: Set the initial eigenpairs as $\mathcal{D} = \begin{bmatrix} X_k^{(0)} \\ \alpha_k^{(0)} \end{bmatrix}$ for k = 1,..., m (some number of

extreme eigenvalues) where $X_k^{(0)}$ is the k-th column of orthogonal matrix V.

Step 3: Compute for k = 1,..., n (in Parallel)

(i) $||(A - \alpha_k^{(0)} I)X_k^{(0)}||_2$.

(ii) If $||(A - \alpha_k^{(0)} I)X_k^{(0)}||_2 < \epsilon, \epsilon = 10^{-8}$, then go to Step 5, otherwise go to Step 3.

Step 4: Apply the modified Newton method.

Modified Newton's Iteration: (in Parallel)

For k=1,2,...,n.

For i=1,...

(i) Solve $(A - \alpha_k^{(i)} I)Y_k^{(i)} = X_k^{(i)}$.

(ii) Compute $\beta_k^{(i)} = (X_k^{(i)})^T Y_k^{(i)}$.

(iii) Compute $\hat{\beta_k} i) = ||Y_k^{(i)}||_2$.

(iv) $X_k^{(i+1)} = \frac{y_k^{(i)}}{\hat{\beta_k} i)}$.

(v) $\alpha_k^{(i+1)} = \alpha_k^{(i)} - \frac{\hat{\beta}}{\beta_k^{(} i)^2}$.

(vi) $\alpha_k^{(i)} -> \alpha_k^{(i+1)}$, $X_k^{(i)} -> X_k^{(i+1)}$.

(vii) Check $||(A - \alpha_k^{(i)} I)X_k^{(i)}||_2 < \epsilon$. Otherwise, go to Step 3 - (i).

Step 5: Let m be the number of eigenpairs obtained from Step 3. If m = n, then all the n eigenpairs are obtained. If m|n, then obtain the (n-m) eigenpairs as follows: Denote by $\{G_k\}_{j=1,\cdots,m}$ the m groups of eigenpairs as defined below. $G_k = \left\{ \begin{bmatrix} X_k^{(0)} \\ \alpha_k^{(0)} \end{bmatrix} \begin{bmatrix} X_k^{(0)} \\ \alpha_k^{(0)} \end{bmatrix} \text{ converges to } \begin{bmatrix} U_k \\ \lambda_k \end{bmatrix} \right\}$ for $k = 1, \cdots, m$ where $m_1 + \cdots + m_m = n$, m_i is the number eigenpairs in each group.

For $k = 1, \cdots, m$ (in Parallel)

(i) Compute $min_{1 \le j \le m_k} ||(A - \alpha_{k_j}^{(0)} I)X_{k_j}^{(0)}||$. (Note that for each group there is one vector which satisfies the above relation.)

(ii) Orthogonalize the other vectors.

For $k = 1, \cdots, m$ (in Parallel):

For $j = 1, \cdots, (m_k - 1)$.

Orthogonalize using $\left\{U_1, U_2, \cdots, U_l, X_{k_j}^{(0)}\right\} \rightarrow \left\{U_1, U_2, \cdots, U_l, \hat{X_{k_j}^{(0)}}\right\}$using the modified Gram-Schmidt process.

(iii) Using Step 3 with eigenpair $\begin{bmatrix} X_k^{(0)} \\ \alpha_k^{(0)} \end{bmatrix}$, obtain a new set of eigenpairs $\begin{bmatrix} X_k^{(i)} \\ \alpha_k^{(i)} \end{bmatrix}$.

(iv) Set $\begin{bmatrix} \hat{X_k^{(0)}} \\ \alpha_k^{(0)} \end{bmatrix} \rightarrow \begin{bmatrix} U_k \\ \lambda_k \end{bmatrix}$.

Step 6: End.

We describe algorithm using the group homotopy method with a choice of Gap^*.

4.2 Algorithm II : Group Homotopy method

Let $A = (a_{ij}) \in M_n$ be a given symmetric matrix with eigenpairs $\begin{bmatrix} U_k \\ \lambda_k \end{bmatrix}$ for $k = 1, \cdots, n$ and $S = diag(\alpha_1^{(0)}, \cdots, \alpha_n^{(0)})$. Consider $A(t_{i+1}) = (1 - t_i)S + t_i A$ where $0 \leq t_i \leq 1$and $\Delta t_i = t_{i+1} - t_i$. Suppose $Gap^* = \delta||A - S||_2$, then $\Delta t_i = \left(\frac{\delta||A-S||_2}{q}\right) \cdot \left(\frac{1}{||A-S||_2}\right) = \frac{\delta}{q}$. In the following algorithm we choose $\delta = 1$ and q = 4 which leads to the step size $\Delta t_i = 0.25$. Consider $A(t_0) = S = diag(\alpha_1^{(0)}, \cdots, \alpha_n^{(0)}$ where diagonal elements of $A(t_0)$ are arranged in decreasing order. Note $A(0) = S$.
Set $t_0 = 0, \Delta t_i = 0.25$.

Step 1 : Choose the initial eigenpairs of $A(0) = \left\{ \begin{bmatrix} X_k^{(0)} \\ \alpha_k^{(0)} \end{bmatrix} \right\}$ for $k = 1, \cdots, n$ where $X_k^{(0)}$ is the k-th column of orthogonal matrix V. Set $t_0 = 0, \Delta t_i = 0.25$.

Step 2 : For i = 1,2,3,4. : (i) $t_i = t_{i-1} + \Delta t$. (ii) Arrange the eigenvalues of $A(t_{i-1})$ in decreasing order with corresponding eigenvectors. (iii) Apply Algorithm I(modified Newton method with orthogonalization) from step 2, to obtain all the eigenpairs of$A(t_i)$. (iv) If $t \neq 1$, go to step 2-(i).

Step 3 : End.

4.3 Numerical Results

Since $\|\cdot\|_2 \leq \|\cdot\|_F$ where $\|\cdot\|_F$ is the Frobenius matrix norm and $\|\cdot\|_F$ is easy to compute, we use $\|A - S\|_F$ to compute Δt_i in the following examples.

M = the number of eigenpairs obtained using the modified Newton iteration.
B = the number of eigenpairs recovered with modified Gram-Schmidt process using the modified Newton iteration.
C = the maximum number of iterations at each step.
D = the maximum number of iterations needed for the orthogonalization.

Example 4.1: Consider the matrix

$$A = [a_{ij}], \in M_n \quad \begin{array}{ll} a_{ij} = i & \text{if } i > j, \\ a_{ij} = (-1)^i 3 * i & \text{if } i = j, \\ a_{ij} = j & \text{if } j > i. \end{array}$$

Choose the initial matrix S such that $A(0) = S = diag(a_{11}, a_{22}, \ldots, a_{nn})$. $\|A - S\|_F = 1779.2$. The result of Table 4.1 uses $q = 4$ in Algorithm II.

Table 4.1 (using Algorithm II, $q = 4$, $n = 50$)

Eigenvalues of $A(t_i)$	t_0 0	t_1 0.25	t_2 0.5	t_3 0.75	t_4 1.0	Exact Eigenvalues
1st	150.00	457.8705	879.5562	1308.3704	1739.0537	1739.0537
⋮	⋮	⋮	⋮	⋮	⋮	⋮
20th	36.00	32.0262	32.6110	27.9100	23.4161	23.4161
⋮	⋮	⋮	⋮	⋮	⋮	⋮
30th	-27.00	-27.6036	-30.4504	-33.3424	-36.2029	-36.2029
⋮	⋮	⋮	⋮	⋮	⋮	⋮
40th	-87.00	94.4645	-96.4081	-104.6880	-112.8265	-112.8265
⋮	⋮	⋮	⋮	⋮	⋮	⋮
50th	-147.00	-164.1900	-215.4465	-285.9817	-363.2445	-363.2445
M		46	44	45	45	
B		4	6	5	5	
C(D)		8(6)	8(5)	10(4)	8(4)	

From the results of numerical experiments below, it is clear that if q is large then the number of iterations in each step is significantly lower (see last row of each table) and also the number of eigenpairs recovered using algorithm I (Step 4) is also less (row representing B).

Example 4.2:

We apply to compute the largest and smallest eigenvalues of symmetric matrices. In order to choose the initial matrix that is close to the largest and smallest eigenvalues of the given matrix, we use the Lanczos method to get a good choice of the initial points.
(1) A symmetric matrix $A = (a_{ij}) \in M_n, a_{ij} = i$ if $i > j$, $a_{ij} = (-1)^i 3 * i$, if $i = j, a_{ij} = j$ if $j > i$. Choose the initial matrix T such that T=$V^T AV$. (see Table 4.2.1)
(2) A symmetric Toeplitz matrix A , $b_i = 2 * i + i$ and the initial matrix T such that T=$V^T AV$. (see Table 4.2.2)

Table 4.2.1

n	extreme eigenvalues	the initial value	Eigenvalues	iterations
50	the smallest	-215.00	-363.2445	8
	the largest	739.00	1739.0537	5
100	the smallest	-1.1641e+003	-1.3400e+003	5
	the largest	6.6690e+003	6.9441e+003	5
200	the smallest	-4.6122e+003	-5.2113e+003	5
	the largest	2.7127e+004	2.7776e+004	5
300	the smallest	-1.1013e+004	-1.1637e+004	5
	the largest	6.1646e+004	6.2505e+004	5
400	the smallest	-1.9315e+004	-2.0617e+004	5
	the largest	1.0999e+004	1.1113e+004	5
500	the smallest	-3.0656e+004	-3.2151e+004	5
	the largest	1.7232e+005	1.7365e+005	5

Table 4.2.2

n	extreme eigenvalues	the initial value	Eigenvalues	iterations
50	the smallest	-1.0095e+003	-1.0135e+003	5
	the largest	1.8774e+003	1.8814e+003	5
100	the smallest	-3.9720e+003	-4.0532e+003	4
	the largest	7.1716e+003	7.2374e+003	4
200	the smallest	-1.618e+004	-1.6212e+004	4
	the largest	2.8196e+004	2.8372e+004	4
300	the smallest	-3.6322e+004	-3.6476e+004	4
	the largest	6.13294e+004	6.3402e+004	4
400	the smallest	-6.4600e+004	-6.4846e+004	4
	the largest	1.1222e+005	1.1233e+005	4
500	the smallest	-1.0103e+005	-1.0132e+005	4
	the largest	1.7502e+005	1.7515e+005	4

Example 4.3:
A symmetric matrix $A = (a_{ij}) \in M_n, a_{ij} = i$ if $i > j$, $a_{ij} = (-1)^i 3 * i$, if $i = j, a_{ij} = j$ if $j > i$. Comparison of the existing method for the largest eigenvalue of the given matrix A.

Table 4.3

n	Power Method	Inverse Power	Rayleigh Quotient	eigenvalue
	iterations	iterations	iterations	
50	6	6	2	1739.0537
100	7	6	2	6.9441e+003
200	8	6	2	2.7776e+004
300	8	6	2	6.2505e+004
400	9	6	2	1.1113e+005
500	9	6	2	1.7365e+005

From Table 4.3, we compare the existing methods(power, inverse power and rayleigh quotient) in the same matrix. In this method, we can compute the largest/smallest eigenvalue at once. If we compute the largest one and the smallest one at once, it is impossible to get them. The procedure is a sequential process. The existing method is limited to get a few of extreme eigenvalues at once. Our method is developed to deal with those drawbacks in the existing methods.

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