

A Note on the Homotopy Method for Linear Algebraic Eigenvalue Problems

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ABSTRACT

Recently the homotopy method has been applied to solve linear algebraic eigenvalue problems. On the basis of theoretical advantages and practical experiments, the method has been suggested as a serious alternative to EISPACK for finding all isolated eigenpairs of large, sparse linear algebraic eigenvalue problems on SIMD machines. This note offers a simpler proof than Li and Sauer's of the existence of homotopy curves for eigenvalue problems of general matrices.

1. INTRODUCTION

Let $A, B \in \mathbb{C}^{n \times n}$ and $\mu \in \mathbb{C}$. Consider the linear algebraic eigenvalue problems

$$Ax = \mu x \tag{1.1}$$

and

$$Ax = \mu Bx. \tag{1.2}$$

We shall assume that the factorization of A and B is either impossible or undesirable, as might be the case if A and B are large and structured. One approach to these problems is to impose an additional normalization condition

$$s^*x = 1, \tag{1.3}$$

and to formulate (1.1) and (1.2), respectively, as systems of $n + 1$ polynomials in $n + 1$ variables (x_1, \dots, x_n, μ) :

$$f(x, \mu) = \begin{bmatrix} \mu x - Ax \\ s^*x - 1 \end{bmatrix} = 0 \quad (1.4)$$

and

$$g(x, \mu) = \begin{bmatrix} \mu Bx - Ax \\ s^*x - 1 \end{bmatrix} = 0. \quad (1.5)$$

Since the higher order Fréchet derivatives can easily be determined, the conventional Newton's methods can be applied to solve these equations [1, 3]. In doing so, it is easy to see that Newton's method amounts to a version of the inverse power method [10, 12]. Unfortunately, Newton's method can converge (if it ever converges) to only one zero at a time. When computing several eigenpairs, one has to restart the iteration either by making suitable initial guesses or by choosing the normalization vector c as a vector orthogonal to those eigenvectors already found [1].

In [2], a homotopy method was proposed by this author to find *all* eigenpairs of (1.1) when A is n by n *real, symmetric, and tridiagonal* with nonzero off-diagonal elements. It was shown that there were exactly n independent smooth curves connecting obvious points to the desired eigenpairs. The homotopy method clearly has the following theoretical advantages:

- (1) All isolated eigenpairs are guaranteed to be reached. The method even can approximate nonisolated eigenpairs.
- (2) The homotopy curves correspond only to different initial values of the same ordinary differential equations. Hence all curves can be followed simultaneously if there are enough processors.
- (3) The symmetric tridiagonal structure remains unchanged under the homotopy transition.

Recently Rhee [9] explored the homotopy method further by showing that the local conditioning of the homotopy curves was affected by two factors only—the separation of eigenvalues of the transition matrix $D + t(A - D)$ and the closeness of D to A , where D is the diagonal matrix (or any other simple matrix) used at $t = 0$. In particular, this implies that the conditioning of the homotopy curve is independent of the size of the matrix. He also developed a numerical algorithm of which test results consistently showed that the overall complexity of the homotopy method for finding all eigenpairs would be $O(n^2)$ as opposed to $O(n^{2.6})$ of the standard subroutine `IMRQL2` in `EISPACK`. All of this evidence seems to suggest that the homotopy method

might be used a serious alternative to EISPACK for finding all eigenpairs of large scale symmetric eigenvalue problems on SIMD machines.

The key issue encountered in applying the continuation method is the selection of an appropriate homotopy equation so that the existence of curves connecting the trivial solution and the desired solutions is assured and so that the numerical work in following these curves is at reasonable cost. It was not clear whether the homotopy proposed in [2] could be applied to solve (1.1) for general matrices. Apparently, the proof given in [2] depends upon the symmetric tridiagonal structure, which seems difficult to generalize.

Recently Li, Sauer, and Yorke [6] proposed a homotopy method for the case when A is a general matrix and B is nonsingular. Li and Sauer further proposed in [5] a homotopy method for the case when B is singular. In both articles, the main idea is to perceive the systems (1.4) and (1.5) to be in the n -dimensional projective space, then to identify the singularity structure of zeros at infinity, and then to construct a homotopy which respects this special structure for all $t \in [0, 1)$. The proofs utilized the concept of the resultant of polynomials [13] to assure that the singularity structure of zeros at infinity remained unchanged throughout the deformation and, finally, a version of Bezout's theorem [4] to count the number of isolated zeros in \mathbb{C}^n .

In this paper, we show that the homotopy equation formed in [2] for tridiagonal symmetric matrices works equally well for general matrices. We also construct a homotopy equation for the problem (1.2) when both A and B are general matrices. The idea in this paper should be credited to Li et al. [5, 6]. But we do not rely on the relatively sophisticated machinery from algebraic geometry. The justification of our homotopy method is based on a rather simpler version of the resultant theorem which will be discussed in the next section. Sections 3 and 4 are then devoted to the analysis of the homotopy equations for (1.1) and (1.2), respectively.

2. PRELIMINARY RESULTS

We first briefly review the concept of the resultant of two polynomials. Let

$$\begin{aligned}
 p(x) &= a_0x^n + a_1x^{n-1} + \dots + a_n, \\
 q(x) &= b_0x^m + b_1x^{m-1} + \dots + b_m
 \end{aligned}
 \tag{2.1}$$

be two polynomials with coefficients a_i and b_j in C . Then the determinant R

$A + D$ has a multiple eigenvalue if and only in the resultant R of $c(\lambda)$ and $c'(\lambda)$ vanishes. Notice that R is not identically zero, since, by the Gershgorin theorem, one may choose the d_i 's far away enough from each other and the origin to make $A + D$ only have simple eigenvalues. Notice also that R is a polynomial in the undetermined variables d_1, \dots, d_n . So, by Theorem 2.2, the set $E = R^{-1}(0)$ has measure zero. Furthermore, R cannot vanish identically in any open set; otherwise R would be identically zero everywhere. This shows that U is dense. ■

A result similar to Theorem 2.3 can also be established for the diagonal perturbation of a matrix pencil (A, B) .

THEOREM 2.4. *Given two arbitrary matrices $A, B \in \mathbb{C}^{n \times n}$ where none of the diagonal elements of B is zero, then the complement U of the set $E = \{(d_1, \dots, d_n) \in \mathbb{C}^n \mid D = \text{diag}(d_1, \dots, d_n) \text{ such that the matrix pencil } (A + D, B) \text{ has multiple eigenvalues}\}$ is open, is dense, and has full Lebesgue measure in \mathbb{C}^n .*

Proof. The proof is almost exactly the same as in Theorem 2.3 except that when showing the resultant is not identically zero we need to apply a generalized Gershgorin-type theorem for the generalized eigenvalue problem. This theory was first established by Stewart in [11]. The nonzero diagonal elements of B are required to ensure the separation of eigenvalues at infinity. Readers are invited to finish the details of the proof. ■

3. THE REGULAR EIGENVALUE PROBLEM

We shall construct a homotopy function $H: \mathbb{C}^n \times \mathbb{C} \times [0, 1] \rightarrow \mathbb{C}^n \times \mathbb{C}$ as follows:

$$H(x, \mu, t) = \begin{bmatrix} \mu x - [D + t(A - D)]x \\ \frac{1}{2}(x^*x - 1) \end{bmatrix}, \tag{3.1}$$

where D is a randomly generated diagonal matrix. Without causing any ambiguity, the homotopy function (3.1) can also be regraded as a mapping $H: \mathbb{R}^{2n} \times \mathbb{R}^2 \times [0, 1] \rightarrow \mathbb{R}^{2n} \times \mathbb{R}$. We are interested in the set $H^{-1}(0)$. Note that $H(x, \mu, 0) = 0$ corresponds to the trivial eigenvalue problem $\mu x = Dx$, and $H(x, \mu, 1) = 0$ corresponds to the problem (1.1).

Let $Q = Q(x, \mu, t)$ be the n by $n + 1$ complex matrix

$$Q(x, \mu, t) = [\mu I - [D + t(A - D)], x]. \quad (3.2)$$

Consider the set $E = \{(d_1, \dots, d_n) \in \mathbb{C}^n; D = \text{diag}(d_1, \dots, d_n) \text{ such that } \tau D + A \text{ has multiple eigenvalues for at least one } \tau \in (0, \infty)\}$. By Theorem 2.3, we know that topologically E is of real codimension one in \mathbb{C}^n . The complement U of E is open, is dense, and has full measure in \mathbb{C}^n . If the elements of D are chosen from U , then the transition matrix $\alpha(t) = D + t(A - D)$ will have simple eigenvalues for all $t \in [0, 1)$.

If $H(x, \mu, t) = 0$, then

$$\alpha(t)x = \mu x. \quad (3.3)$$

We claim

LEMMA 3.1. *If $H(x, \mu, t) = 0$ for some $t \in [0, 1)$, then the n by $n + 1$ complex matrix $Q = Q(x, \mu, t)$ is of complex rank n .*

Proof. Let P be the nonsingular matrix such that

$$P^{-1}(t)[\mu I - \alpha(t)]P(t) = J(t), \quad (3.4)$$

where $J(t)$ is the Jordan canonical form of $\mu I - \alpha(t)$. Since $\alpha(t)$ has only simple eigenvalues for $t \in [0, 1)$, $J(t)$ actually is a diagonal matrix. The rank condition for the matrix $Q(x, \mu, t)$ is the same as that for the matrix

$$G(x, \mu, t) = [J(t), P^{-1}(t)x]. \quad (3.5)$$

Without loss of generality, we may assume the $(1, 1)$ component of G is zero. Since x is proportional to the first column of the matrix P , the column vector $P^{-1}x$ must be of the form $P^{-1}x = [c, 0, \dots, 0]^T$ for some nonzero complex number c . It follows that the matrix Q is of complex rank n . ■

Recall that a linear transformation from \mathbb{C}^{n+1} to \mathbb{C}^n can be regarded as a linear transformation from \mathbb{R}^{2n+2} to \mathbb{R}^{2n} if each component, say $z = a + ib$, of the complex matrix is replaced by the 2 by 2 real matrix

$$\begin{bmatrix} a & -b \\ b & a \end{bmatrix}.$$

Let $\hat{Q} = \hat{Q}(x, \mu, t)$ denote the $2n$ by $2n + 2$ real matrix associated with the n by $n + 1$ complex matrix Q . Suppose each component x_k of the complex vector x is written as $x_k = a_k + ib_k$. Define the $2n + 1$ by $2n + 2$ real matrix $M = M(x, \mu, t)$ as follows:

$$M(x, \mu, t) = \begin{bmatrix} & & & \hat{Q} & & \\ a_1, & b_1, & a_2, & \dots, & a_n, & b_n, & 0, & 0 \end{bmatrix}. \tag{3.6}$$

We claim

LEMMA 3.2. *If $H(x, \mu, t) = 0$ for some $t \in [0, 1)$, then the $2n + 1$ by $2n + 2$ real matrix $M = M(x, \mu, t)$ is of real rank $2n + 1$.*

Proof. If $H(x, \mu, t) = 0$, then, by (3.3), the last row of M is orthogonal to all other rows of M . The assertion follows now from Lemma 3.1. ■

Regarding the homotopy function H as the one defined in the real space, we now summarize our major results in the following theorem.

THEOREM 3.3. *There exists an open dense set U with full Lebesgue measure in \mathbb{C}^n such that if $d = \text{diag}(d_1, \dots, d_n)$ with $(d_1, \dots, d_n) \in U$, then:*

(1) *The zero set $H^{-1}(0) = \{(x, \mu, t) | H(x, \mu, t) = 0 \text{ for some } t \in [0, 1)\}$ with H defined by (3.1) is a 2-dimensional smooth submanifold in $\mathbb{R}^{2n} \times \mathbb{R}^2 \times \mathbb{R}$.*

(2) *$H^{-1}(0)$ is uniformly bounded and hence is extendable to $t = 1$.*

Proof. The first part follows immediately from Lemma 3.2 and the implicit function theorem. It only remains to show the uniform boundedness of $H^{-1}(0)$. To see this, observe that for any $(x, \mu, t) \in H^{-1}(0)$ we have $\|(x, \mu, t)\| \leq 2 + |\mu|$. But from (3.3), it is clear that $|\mu| \leq \|D\| + \|A\|$. The continuity then assures that this uniform bound still holds when $t \rightarrow 1$. ■

REMARK 3.4. For $i = 1, \dots, n$, let e_i represent the i th standard unit vector in \mathbb{R}^n . It is obvious that $y_i = (e_i, d_i, 0) \in H^{-1}(0)$. Let $C(y_i)$ denote the component of y_i in $H^{-1}(0)$. Since $H(x, \mu, t) = 0$ implies $H(\gamma x, \mu, t) = 0$ whenever $\gamma \in \mathbb{C}$ and $|\gamma| = 1$, $C(y_i)$ indeed is a 2-dimensional cylindrical tube whose cross section with each hyperplane $t \equiv \text{constant} \in [0, 1)$ is a unit circle centered at $(0, \mu) \in \mathbb{R}^{2n} \times \mathbb{R}^2$ for some μ . The implicit function theorem and Lemma 3.2 guarantee that this circle can be continued in both positive and negative directions of t .

We now show how to extract a path from the tube $C(y_i)$ that could be followed numerically and would lead from $t=0$ to $t=1$. According to Remark 3.4, we may require further that this path to be parametrized by the variable t . Among the many possible ways to define such a path, we find the integral curve of the vector field satisfying the following conditions appears to be easier to implement: If H is considered as a mapping from $\mathbb{R}^{2n} \times \mathbb{R}^2 \times [0, 1]$ to $\mathbb{R}^{2n} \times \mathbb{R}$, so that (x, μ) is identified as a vector in $\mathbb{R}^{2n} \times \mathbb{R}^2$ and $(A - D)x$ and ix as vectors in \mathbb{R}^{2n} , then

$$M(x, \mu, t) \begin{bmatrix} \dot{x} \\ \dot{\mu} \end{bmatrix} = \begin{bmatrix} (A - D)x \\ 0 \end{bmatrix}, \tag{3.7}$$

$$[ix^T, 0] \begin{bmatrix} \dot{x} \\ \dot{\mu} \end{bmatrix} = 0. \tag{3.8}$$

The last equation (3.8) simply means the vector field is always perpendicular to the circle of the intersection of the hyperplane $t \equiv \text{constant}$ and the tube. The $2n + 2$ by $2n + 2$ real matrix

$$\begin{bmatrix} M(x, \mu, t) \\ ix^T, 0 \end{bmatrix} = \begin{bmatrix} \hat{Q}(x, \mu, t) \\ a_1, b_1, \dots, a_n, b_n, 0, 0 \\ -b_1, a_1, \dots, -b_n, a_n, 0, 0 \end{bmatrix}$$

is precisely the real representation of the $n + 1$ by $n + 1$ complex matrix

$$\begin{bmatrix} \mu I - [D + t(A - D)], & x \\ x^*, & 0 \end{bmatrix}.$$

Therefore, the remaining numerical work amounts to solving the following initial value problems in $\mathbb{C}^n \times \mathbb{C}$:

$$\begin{bmatrix} \mu I - [D + t(A - D)], & x \\ x^*, & 0 \end{bmatrix} \begin{bmatrix} \dot{x} \\ \dot{\mu} \end{bmatrix} = \begin{bmatrix} (A - D)x \\ 0 \end{bmatrix}, \tag{3.9}$$

$$x(0) = e_i, \quad \mu(0) = d_i$$

for $i = 1, \dots, n$.

REMARK 3.5. Let k_a and k_g represent the algebraic and geometric multiplicities of an eigenvalue μ of A , respectively. Let x be a corresponding normalized eigenvector of μ .

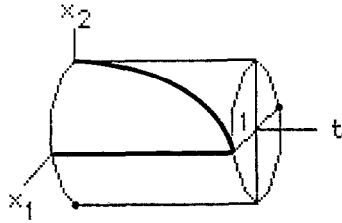


FIG. 1. $A = \begin{pmatrix} 2 & 1 \\ 0 & 2 \end{pmatrix}$.

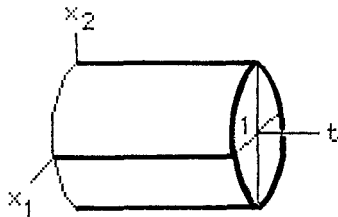


FIG. 2. $A = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$.

(1) If $k_a = k_g = 1$, i.e. if (x, μ) is an absolutely isolated eigenpair of A , then it is easy to see that the corresponding matrix $G(x, \mu, 1)$ is still of full complex rank. So the integral curve determined by (3.9) passes through the hyperplane $t \equiv 1$ transversely.

(2) If $k_a = 2$, then the matrix of the right-hand side of (3.9) is necessarily singular. But according to Theorem 3.3, the curve determined by (3.9) for $t < 1$ can always be extended to reach $t = 1$. Figures 1 and 2 exemplify, respectively, the projections of $H^{-1}(0)$ into the space of $(x, t) \in \mathbb{R}^2 \times [0, 1]$ for the cases $k_g = 1$ and $k_g = 2$.

4. THE GENERALIZED EIGENVALUE PROBLEM

For the generalized eigenvalue problem (1.2), we shall construct a homotopy function $H: \mathbb{C}^n \times \mathbb{C} \times [0, 1] \rightarrow \mathbb{C}^n \times \mathbb{C}$ as follows:

$$H(x, \mu, t) = \begin{bmatrix} [(1-t)(c\mu I - D) + t(\mu B - A)]x \\ \frac{1}{2}(x^*x - 1) \end{bmatrix}, \tag{4.1}$$

where $c \in \mathbb{C}$ and $D = \text{diag}(d_1, \dots, d_n)$ are randomly generated. Note that $H(x, \mu, 0) = 0$ corresponds to the trivial problem $c\mu x = Dx$, and $H(x, \mu, 1)$ corresponds to the problem (1.2). Let $\beta(t) = (1-t)cI + tB$ and $\alpha(t) = (1-t)D + tA$.

It is easy to see that there exists an open dense set V in \mathbb{C} such that if $c \in V$, then $\beta(t)$ is nonsingular and has no zero diagonal elements for each $t \in [0, 1)$. We shall assume henceforth that $c \in V$.

Let $Q = Q(x, \mu, t)$ be the n by $n+1$ complex matrix

$$Q(x, \mu, t) = [\beta(t)\mu - \alpha(t), \beta(t)x]. \quad (4.2)$$

Consider the set $E = \{(d_1, \dots, d_n) \in \mathbb{C}^n; D = \text{diag}(d_1, \dots, d_n) \text{ such that } [\beta(t)]^{-1}\alpha(t) \text{ has multiple eigenvalues for at least one } t \in [0, 1)\}$. It follows again from Theorem 2.4 that topologically E is of real codimension one in \mathbb{C}^n . Therefore, the complement U of E is open, is dense, and has full measure in \mathbb{C}^n . If the diagonal elements of D are chosen from U , then for $0 \leq t < 1$ and for any μ the matrix $\beta(t)\mu - \alpha(t)$ can have at most one zero eigenvalue.

If $H(x, \mu, t) = 0$, then x will be an eigenvector of $\beta(t)\mu - \alpha(t)$ associated with the simple eigenvalue 0. From now on all the discussions are analogous to those in the previous section. In particular, the matrix $Q(x, \mu, t)$ is of complex rank n . Without repeating the proof, we summarize our results in the following theorem:

THEOREM 4.1. *There exists an open dense set U with full Lebesgue measure in \mathbb{C}^n and an open dense set V in \mathbb{C} such that if $c \in V$ and if $D = \text{diag}(d_1, \dots, d_n)$ with $(d_1, \dots, d_n) \in U$, then:*

(1) *The zero set $H^{-1}(0) = \{(x, \mu, t) | H(x, \mu, t) = 0 \text{ for some } t \in [0, 1)\}$ with H defined by (4.1) is a 2-dimensional smooth submanifold in $\mathbb{R}^{2n} \times \mathbb{R}^2 \times \mathbb{R}$.*

(2) *The solution to the initial value problems in $\mathbb{C}^n \times \mathbb{C}$*

$$\begin{bmatrix} \beta(t)\mu - \alpha(t) & \beta(t)x \\ x^* & 0 \end{bmatrix} \begin{bmatrix} \dot{x} \\ \dot{\mu} \end{bmatrix} = \begin{bmatrix} [\mu(cI - B) + (A - D)]x \\ 0 \end{bmatrix}, \quad (4.3)$$

$$x(0) = e_i, \quad \mu(0) = d_i/c$$

for $i = 1, \dots, n$ characterize n smooth curves on the set $H^{-1}(0)$.

REMARK 4.2. The following are discussions of the behavior of curves defined by (4.3) as $t \rightarrow 1$. We shall exclude the two extreme cases where

either $\det(\mu B - A) \equiv 0$ or $\det(\mu B - A) \equiv$ nonzero constant. In the former case, every complex value is an eigenvalue of the problem (1.2). In the latter case, the problem (1.2) has no eigenvalue at all.

(1) Suppose that B is nonsingular. Then $\beta(t)$ is continuous and nonsingular for all $t \in [0, 1]$. If $H(x, \mu, t) = 0$, let $\phi(t) = \|\beta(t)x(t)\|$. Obviously $\phi([0, 1])$ is a compact subset not containing 0. Since $|\mu| \leq \|\alpha(t)\|/\|\beta(t)x(t)\|$, we have shown that the set $H^{-1}(0)$ is uniformly bounded. Furthermore, a discussion analogous to that made in the previous section can be given. In particular, it can be shown now that each isolated eigenvector of (1.2) will be reached by at least one homotopy curve in $H^{-1}(0)$.

(2) Suppose that B is singular. Then some of the curves defined by (4.3) will blow up as $t \rightarrow 1$. But still it can be shown that each isolated eigenvector of (1.2) must be reached by at least one homotopy curve.

5. CONCLUSIONS

The homotopy method can be applied to solve the linear algebraic eigenvalue problems for general matrices. The two special homotopy equations (3.1) and (4.1) are constructed for the problems (1.1) and (1.2), respectively. We have shown that in either case the zero set $\{(x, \mu, t) \in \mathbb{C}^n \times \mathbb{C} \times [0, 1]; H(x, \mu, t) = 0\}$ is a 2-dimensional smooth manifold. Homotopy curves on the zero set can be defined by the initial value problems (3.9) and (4.3), respectively. We also have shown that each isolated eigenvector together with its corresponding eigenvalue is connected by at least one of these homotopy curves. In fact, each *isolated eigenpair* is connected transversely by a unique homotopy curve.

Since the homotopy curves correspond only to different initial values of the same ordinary differential equations, the independence of these curves makes it feasible to follow several curves simultaneously on a multiprocessor machine. Note also that the homotopy equations constructed in (3.1) and (4.1) do not cause any destruction of the matrix structure of A or B . Together with sparse matrix techniques, the homotopy method therefore might become attractive for solving large scale linear algebraic eigenvalue problems.

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