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Verified numerical computations for multiple or nearly multiple eigenvalues for elliptic operators

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Abstract

In this paper, we propose a numerical method to verify multiple eigenvalues for elliptic eigenvalue problems. We calculate error bounds for approximations of multiple eigenvalues and base functions of the corresponding invariant subspaces. For matrix eigenvalue problems, Rump [1] recently proposed a validated numerical method to compute multiple eigenvalues. In this paper, we extend his formulation to elliptic eigenvalue problems, combining it with a method developed by one of the authors [2].

1 Introduction

A method is proposed to enclose the eigenvalues and eigenfunctions for the elliptic eigenvalue problems by using the numerical verification method for nonlinear elliptic problems. But the method can only be applied to the simple eigenvalues according to the verification principle. Namely, applying the method for multiple eigenvalues leads to a singularity due to the multiplicity. For the matrix eigenvalue problems, a method to compute the error bounds for the approximations of multiple or nearly multiple eigenvalues, and to verify a basis of the corresponding invariant subspaces was proposed in [1].

In this paper, we try to extend this formulation to the elliptic eigenvalue problems. In order to attain our present purpose, we use the basic idea same as in the numerical verification method for elliptic problems. We formulate the multiple eigenvalue problem for elliptic operator as a system of nonlinear elliptic boundary value problem with respect to the eigenvalues and the base functions of the corresponding invariant subspace. Then, by applying a kind of set valued Newton's method, we enclose those quantities in computer.

We use an approximation subspace to compute the finite dimensional part of the problem, and by using the constructive error estimates we enclose the infinite dimensional part. In the present case, we adopt the spectral method based on the Fourier series expansion and the explicit a priori error estimates.

In the following section, we describe the basic formulation of the problem and the actual computational procedures for selfadjoint case.

Our method enables us not only to enclose eigenvalues but also to verify a basis of the corresponding invariant subspaces.

2 Formulation of the problem

We define Ω as a bounded convex domain in R^2. Let $H^m(\Omega)$ denote the L^2-Sobolev space of order m on Ω for an integer m, and we define $H_0^1 \equiv H_0^1(\Omega) \equiv \{v \in H^1(\Omega) | v = 0 \text{ on } \partial\Omega\}$ and the inner product on H_0^1 as $< u, v >_{H_0^1} \equiv (\nabla u, \nabla v)_{L^2}$ for $u, v \in H_0^1(\Omega)$, where $(\cdot,\cdot)_{L_2}$ represents the inner product on $L^2(\Omega)$. Next, let S_h be a finite dimensional subspace of H_0^1, and let $\{\phi_i\}_{i=1\cdots N}$ be a basis in S_h. Let $P_{h1} : H_0^1(\Omega) \to S_h$ denote the H_0^1 -projection defined by

$$(\nabla u, \nabla v)_{L^2} = (\nabla P_{h1} u, \nabla v)_{L^2} \qquad for\ all\ v \in S_h.$$

We basically consider the elliptic eigenvalue problem of the following self-adjoint type

$$\left\{ \begin{array}{rcll} -\Delta u + qu & = & \lambda u & in \quad \Omega, \\ u & = & 0 & on \quad \partial\Omega \end{array} \right. \tag{1}$$

where $q \in L^\infty(\Omega)$.

First we calculate approximate spectrum of (1), and then compute the error bounds for the multiple eigenvalues and cnclose a basis of the corresponding invariant subspace around the approximate solutions.

For matrix eigenvalue problems, Rump [1] shows that error bounds for k-fold computed eigenvalues and the approximate basis of corresponding invarient subspace of $n \times n$ matrix A are calculated by verifing Y, M which satisfy the equation $AY = YM$, where Y is an $n \times k$ matrix and M a $k \times k$ matrix, respectively.

Therefore, in order to extend the method in [1] to the elliptic eigenvalue problem, we transform (1) to the eigen-equation of the form:

$$(-\Delta + q)Y = YM, \tag{2}$$

where $Y \equiv (y_1, y_2, \cdots, y_n)$, and $M \equiv \begin{pmatrix} m_{11} & \dots & m_{1n} \\ \vdots & & \vdots \\ m_{n1} & \dots & m_{nn} \end{pmatrix}$,

and the righthand side of (2) is interpreted as $(YM)_i \equiv \sum_{j=1}^{n} m_{ji} y_j, (1 \leq i \leq n)$ and n is the potential multiplicity, and $y_i \in H_0^1$, and $m_{ij} \in R$.

Then, note that each eigenvalue of M is also the eigenvalue of (1). Here $\{y_i\}_{i=1\cdots n}$ is a basis of the corresponding invarient subspace if they are linearly independent. In this paper, since we try to verify multiple eigenvalues with associated base functions of the corresponding invarient subspace, when a concerned eigenvalue λ is a potential n-fold eigenvalue, taking the space $V \equiv (H_0^1)^n \times (R)^{n^2}$, and we'll verify $(Y, M) \in V$ satisfing (2). We define the inner product on V, for $w_1 = (y_1^1, \cdots, y_n^1, r_1, \cdots, r_{n^2})$ and $w_2 = (y_1^2, \cdots, y_n^2, s_1, \cdots, s_{n^2})$, as below

$$< w_1, w_2 >=< y_1^1, y_1^2 >_{H_0^1} + \cdots + < y_n^1, y_n^2 >_{H_0^1} + r_1 s_1 + \cdots + r_{n^2} s_{n^2}.$$

And for $V_h \equiv (S_h)^n \times (R)^{n^2}$ we define the projection $P_h : V \to V_h$ by

$$P_h(u_1, \cdots, u_n, r_1, \cdots, r_{n^2}) = (P_{h1}u_1, \cdots, P_{h1}u_n, r_1, \cdots, r_{n^2})$$

where $u_i \in H_0^1, (1 \leq i \leq n)$ and $r_j \in R, (1 \leq j \leq n^2)$.

Let $\lambda_i^h \in R, y_i^h \in S_h$ $(1 \leq i \leq n)$ be appropriately approximate solutions of (1) or (2). We now suppose, for each i, that y_i^h is represented as $y_i^h = \sum_{i=1}^{N} c_{ij}\phi_j$, $c_{ij} \in R$. Then, for each i, let $\tilde{\phi}_i$ be the base function whose coefficient takes the maximal value in $\{|c_{i1}|, \cdots, |c_{iN}|\}$.

Thus, we obtain the normalized eigenvalue problem of the form :

$$\begin{cases} (-\Delta + q)(y_1, y_2, \cdots, y_n) = (y_1, y_2, \cdots, y_n) \begin{pmatrix} m_{11} & \dots & m_{1n} \\ \vdots & & \vdots \\ m_{n1} & \dots & m_{nn} \end{pmatrix}, \\ (y_i, \tilde{\phi}_j) = (y_i^h, \tilde{\phi}_j), \; 1 \leq i, j \leq n, \end{cases} \tag{3}$$

which is considered as a kind of the nonlinear system, with respect to y_i and m_{ij} of elliptic equations.

3 Transformation to the fixed point form

We set $y_i = y_i^h + \tilde{y}_i$ and $m_{ij} = m_{ij}^h + \widetilde{m_{ij}}$ in (3) with $m_{ii}^h = \lambda_i^h, m_{ij}^h = 0 (i \neq j)$. Then $\tilde{y}_i$ and $\widetilde{m_{ij}}$ correspond to the errors of the approximate solutions y_i^h and m_{ij}^h, respectively. We'll verify y_i and m_{ij} satisfing (3) by enclosing $\tilde{y}_i$ and $\widetilde{m_{ij}}$. We can rewrite (3) for $w = (\tilde{y}_1, \cdots, \tilde{y}_n, \widetilde{m_{11}}, \cdots, \widetilde{m_{nn}})$, as follows.

$$
\left\{ \begin{array}{rcl}
-\Delta \widetilde{y_1} \equiv f_1(w) & = & (m_{11}^h + \widetilde{m_{11}} - q)\widetilde{y_1} + (m_{21}^h + \widetilde{m_{21}})\widetilde{y_2} + \cdots \\
& & + (m_{n1}^h + \widetilde{m_{n1}})\widetilde{y_n} + \widetilde{m_{11}} y_1^h + \cdots + \widetilde{m_{n1}} y_n^h + v_0^1, \\
& \vdots & \\
-\Delta \widetilde{y_n} \equiv f_n(w) & = & (m_{1n}^h + \widetilde{m_{1n}})\widetilde{y_1} + (m_{2n}^h + \widetilde{m_{2n}})\widetilde{y_2} + \cdots \\
& & + (m_{nn}^h + \widetilde{m_{nn}} - q)\widetilde{y_n} + \widetilde{m_{1n}} y_1^h + \cdots + \widetilde{m_{nn}} y_n^h + v_0^n, \\
(\tilde{y}_i, \tilde{\phi}_j) & = & 0, \ (1 \leq i, j \leq n),
\end{array} \right. \tag{4}
$$

where we defined the residual error v_0^i, for each $1 \leq i \leq n$, by

$$v_0^i = \Delta y_i^h + (m_{ii}^h - q) y_i^h + m_{1i}^h y_1^h + m_{2i}^h y_2^h + \cdots + m_{ni}^h y_n^h.$$

Here we assumed that $S_h \subset H_0^1 \cap H^2$. Using the map on V

$$F(w) \equiv (\ K f_1(w), \cdots, K f_n(w), \widetilde{m_{11}} + (\tilde{y}_1, \tilde{\phi}_1), \cdots, \widetilde{m_{nn}} + (\tilde{y}_n, \tilde{\phi}_n)\ ), \tag{5}$$

where K is the solution operator for the Poisson equation with the homogeneous boundary condition, we have the fixed point equation

$$w = F(w). \tag{6}$$

Now, we decompose (6) into the finite dimensional part and the infinite one as follows:

$$
\left\{ \begin{array}{rcl}
P_h w & = & P_h F(w), \\
(I - P_h) w & = & (I - P_h) F(w).
\end{array} \right.
$$

Next, we use a Newton-like method for the finite dimensional part as below

$$N_h(w) := w_h - [I - P_h F'(0)]_h^{-1} (w_h - P_h F(w)).$$

and we define $T(w) := N_h(w) + (I - P_h)F(w)$. Then, the following eqivalence relation holds.

$$w = T(w) \Longleftrightarrow w = F(w).$$

In what follows, for the sake of simplicity, but without loss of generality, we consider only the case of $n = 2$, i.e., two-fold eigenvalue.

We use Banach's fixed point theorem to verify the solution of $w = T(w)$. We try to find a set W, referred as a 'candidate set', which satisfies the condition of the fixed point theorem.

We decompose a candidate set as $W = W_h \oplus W_\perp$, where $W_h \subset V_h$, and $W_\perp \subset V_h^\perp$. Here, $V_h^\perp$ is the orthogonal complement of V_h in the space V. We consider the candidate set of the form,

$$\begin{aligned} &W_h = (\sum_{i=1}^{N} \mathcal{W}_i\phi_i, \sum_{i=N+1}^{2N} \mathcal{W}_i\phi_i, \mathcal{W}_{2N+1}, \mathcal{W}_{2N+2}, \mathcal{W}_{2N+3}, \mathcal{W}_{2N+4}), \\ &W_\perp = ([\alpha], [\beta], 0, 0, 0, 0), \text{where for } \alpha \in R^+, [\alpha] \equiv \{v \in S_h^\perp \mid \|v\|_{H_0^1} \le \alpha\}, \\ &\text{with intervals, } \mathcal{W}_i = [-W_i, W_i], \ (1 \le i \le 2N+4), \end{aligned} \tag{7}$$

where $S_h^\perp$ denote the orthogonal complement of S_h in H_0^1.

Let T' be the Fréchet derivative of T. Then the verification condition by using the Banach fixed point theorem is conceptually described as

$$T(0) + T'(W)W \subset W.$$

Here,

$$T'(W)W := \{v \in V \mid v = T'(\tilde{w})w, \ \tilde{w}, w \in W\}.$$

We now present a computable verification condition.

Let denote $(I - P_h)T(0)$ and $(I - P_h)T'(W)W$ by $T_\perp(0)$ and $T'_\perp(W)W$, respectively and, for an element $w_\perp = (w_1, w_2, 0, 0, 0, 0) \in V_h^\perp$, set $(w_\perp)_i := w_i, i = 0, 1$. And for an element $\Phi_h \in V_h$ or a set $\Phi_h \subset V_h$ of the form $\Phi_h = (\sum_{i=1}^{N} \mathcal{A}_i\phi_i, \sum_{i=N+1}^{2N} \mathcal{A}_i\phi_i, \mathcal{A}_{2N+1}, \cdots, \mathcal{A}_{2N+4})$, we set $(\Phi_h)_i \equiv \mathcal{A}_i, (1 \le i \le 2N+4)$, which is sometimes called a coefficient vector for Φ_h. Then, we try to find the $2N+6$ dimensional vectors Y, Z, whose components $Y_i > 0$ and $Z_i \ge 0, (1 \le i \le 2N+6)$, satisfying

$$
\begin{aligned}
&(P_h T(0))_i \in \mathcal{Y}_i \\
&\|(T_\perp(0))_1\|_{H_0^1} \le Y_{2N+5} \\
&\|(T_\perp(0))_2\|_{H_0^1} \le Y_{2N+6}
\end{aligned}
\tag{8}
$$

and

$$
\begin{aligned}
&(P_h T'(W)W)_i \subset \mathcal{Z}_i \\
&\|(T'_\perp(W)W)_1\|_{H_0^1} \le Z_{2N+5} \\
&\|(T'_\perp(W)W)_2\|_{H_0^1} \le Z_{2N+6}
\end{aligned}
\tag{9}
$$

where $\mathcal{Y}_i = [-Y_i, Y_i]; \mathcal{Z}_i = [-Z_i, Z_i], (1 \le i \le 2N+4)$, and for a set Φ, define $\|\Phi\|_{H_0^1} \equiv \sup_{\phi \in \Phi} \|\phi\|_{H_0^1}$. Furthermore, we define

$$
\begin{aligned}
\Theta(W) = \{v \in V \quad | \quad & (P_h v)_i \le Y_i + Z_i, 1 \le i \le 2N+4, \\
& \|((I - P_h)v)_1\|_{H_0^1} \le Y_{2N+5} + Z_{2N+5}, \\
& \|((I - P_h)v)_2\|_{H_0^1} \le Y_{2N+6} + Z_{2N+6} \ \}.
\end{aligned}
$$

Then, we can present the verification conditions as follows

Theorem 1. *If $\Theta(W) \subset W$ holds, for a candidate set W in* (6), *namely, for Y_i and Z_i satisfying* (8) *and* (9),

$$
Y_i + Z_i \le W_i, \ \ 1 \le i \le 2N+6
$$

hold, where $W_{2N+5} = \alpha$, $W_{2N+6} = \beta$, then there exists a solution to (6) *in $\Theta(W)$. Moreover, this solution is unique within the set W.*

4 Numerical examples

Example 1:

We considered the following problem.

$$\begin{cases} -\Delta u + \sin(x)\sin(y)u &= \lambda u \quad in\ \Omega, \\ \qquad\qquad u &= 0 \quad on\ \partial\Omega, \quad \Omega = (0,\pi)\times(0,\pi). \end{cases} \tag{10}$$

We consider the following finite-dimensional subspace, ($\mathcal{N} = 11$) in Lemma 1,

$$S_h = \mathrm{span}\{2/\pi \sin(ix)\sin(jy) \mid 1 \le i,j \le 11\}.$$

Let $\lambda_h \in R$ and $y_h \in S_h$ be the Galerkin approximate solutions of (10) defined by

$$(\nabla y_h, \nabla v) + (\sin(x)\sin(y)y_h, v) = (\lambda_h y_h, v) \quad \text{for all } v \in S_h.$$

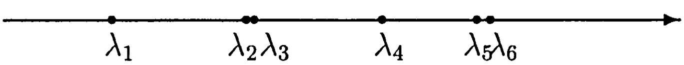

Figure 1: approximate eigenvalues.

We numerically determined approximate eigenvalues for (10). The first eigenvalue was found to be $\lambda_1 \approx 2.71513$. This is seen to be simple. The second and third eigenvalues were found to be $\lambda_2 \approx 5.572374582086$ and $\lambda_3 \approx 5.572374582086$. These eigenvalues are depicted in Figure 1. The numerically determined approximate eigenfunctions y_h^1 and y_h^2 are illustrated in Figures 2 and 3, respectively.

These two eigenvalues seemed to be two-fold or clustered eigenvalues. Therefore, we verified them and the basis of the corresponding invariant subspace around the approximate solutions using the algorithm described in the previous section.

The normalized eigen-equation in question is the following.

$$\begin{cases} (-\Delta + q)(y_1, y_2) &= (y_1, y_2)\begin{pmatrix} m_{11}, m_{12} \\ m_{21}, m_{22} \end{pmatrix}, \\ (y_1, \tilde{\phi}_1) &= (y_1^h, \tilde{\phi}_1), \\ (y_2, \tilde{\phi}_1) &= (y_2^h, \tilde{\phi}_1), \\ (y_1, \tilde{\phi}_2) &= (y_1^h, \tilde{\phi}_2), \\ (y_2, \tilde{\phi}_2) &= (y_2^h, \tilde{\phi}_2). \end{cases}$$

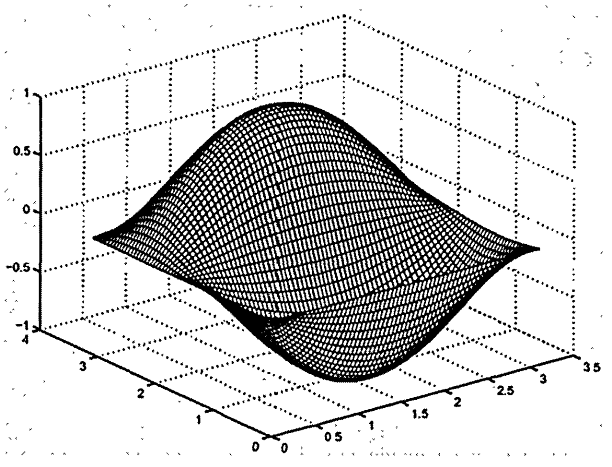

Figure 2: Approximate eigenfunction y_1^h.

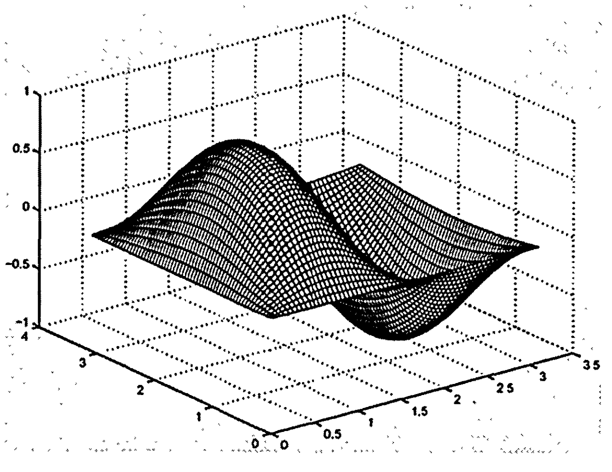

Figure 3: Approximate eigenfunction y_2^h.

Here, $\tilde{\phi}_i$ is taken to be the base function described in Section 2.1. Then, as discussed in Section 2.2, we set $y_i = y_i^h + \tilde{y}_i$ and $m_{ij} = m_{ij}^h + \widetilde{m_{ij}}$ $(1 \le i, j \le 2)$ with $m_{ii}^h = 5.572374582086, m_{ij}^h = 0$ $(i \ne j)$.

The verification results are as follows.
First, the residual errors obtained are $\|v_0^1\|_{L_2} = 0.00489$ and $\|v_0^2\|_{L_2} = 0.00489$. Equations (11) and (12) give the error bounds of the finite-dimensional part of the error from the base functions, i.e., the coefficient vector of $P_{h1}\tilde{y}_i$ $(i = 1, 2)$ in the corresponding invariant subspaces. (13) gives the H_0^1 error bounds of the infinite-dimensional part, i.e., $(I - P_{h1})\tilde{y}_i$ $(i = 1, 2)$:

$$\max(|(Y+Z)_j|) = 0.0905 \times 10^{-4}, \quad 1 \le j \le 11^2, \tag{11}$$
$$\max(|(Y+Z)_j|) = 0.1071 \times 10^{-4}, \quad 11^2 + 1 \le j \le 2 \times 11^2, \tag{12}$$

$$\begin{aligned} \alpha &= 3.6023 \times 10^{-4}, \\ \beta &= 4.3229 \times 10^{-4}. \end{aligned} \tag{13}$$

The elements of the matrix $M = (m_{ij})$ were enclosed as described in (14). The eigenvalues of M were enclosed by using Gerschgorin circles as given in (15): In this example, verification succeeded after 4 iterations , and we used the value 0.1 for the inflation parameter δ in the algorithm.

$$\begin{aligned} m_{11} &\in 5.5724 + [-0.2217, 0.2217] \times 10^{-4}, \\ m_{12} &\in [-0.2550, 0.2550] \times 10^{-4}, \\ m_{21} &\in [-0.2217, 0.2217] \times 10^{-4}, \\ m_{22} &\in 5.5724 + [-0.2550, 0.2550] \times 10^{-4}. \end{aligned} \tag{14}$$

$$\lambda_2, \lambda_3 \in 5.5724 + [-0.4767, 0.4767] \times 10^{-4}. \tag{15}$$

We next numeirally determined the fourth eigenvalue to be $\lambda_4 \approx 8.4581$ 45330119 and found that it is simple. Then we attempt to verify two eigenvalues λ_5 and λ_6 to be close together. Approximate solutions of λ_5 and λ_6 were 10.524940396607 and 10.584986363725, respectively. In this verification procedure, we used the finite dimensional subspace such as

$$S_h = \text{span}\{2/\pi \sin(ix)\sin(jy) \mid 1 \le i, j \le 8\}. \tag{16}$$

The verification results are as follows. The residual errors are $\|v_0^1\| = 0.01339$, and $\|v_0^2\| = 0.01622$.Equations(17) and (18) give the error bounds of the finite-dimensional part of the base functions, i.e., the coefficient vector of $P_{h1}\tilde{y}_i$ $(i = 1, 2,)$ in the corresponding invariant subspaces. (19) gives the H_0^1 error bounds of the infinite-dimensional part, i.e., $(I - P_{h1})\tilde{y}_i$ $(i = 1, 2)$.

$$\max(|(Y + Z)_j|) = 0.0567 \times 10^{-3}, \quad 1 \le j \le 8^2, \tag{17}$$
$$\max(|(Y + Z)_j|) = 0.1032 \times 10^{-3}, \quad 8^2 + 1 \le j \le 2 \times 8^2, \tag{18}$$

$$\begin{aligned} \alpha &= 0.0020, \\ \beta &= 0.0036. \end{aligned} \tag{19}$$

The eigenvalues of M were enclosed by using Gerschgorin circles as follows. In this case verification succeeded after 5 iterations with inflation parameter δ=0.1. As seen in (21) and (22), we were able to enclose two distinct eigenvalues. However, note that when we attempted to verify λ_5 and λ_6 separately as two simple eigenvalues, applying a method similar to that in [2] with the same approximation space S_h, the verification failed.
In the application of the present algorithm, the condition number of the matrix used there, was 121.51. Contrastingly using the method for simple eigenvalues, this quantity became as large as $\approx 3 \times 10^3$. This fact demonstrates the difference between the performances of the two enclosure methods.

$$\begin{aligned} m_{11} &\in 10.584986363725 + [-0.2117, 0.2117] \times 10^{-3}, \\ m_{12} &\in [-0.3745, 0.3745] \times 10^{-3}, \\ m_{21} &\in [-0.2053, 0.2053] \times 10^{-3}, \\ m_{22} &\in 10.524940396607 + [-0.3632, 0.3632] \times 10^{-3} \end{aligned} \tag{20}$$

$$\lambda_5 \in 10.524940396607 + [-0.5685, 0.5685] \times 10^{-3}. \tag{21}$$
$$\lambda_6 \in 10.584986363725 + [-0.5862, 0.5862] \times 10^{-3}. \tag{22}$$

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