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Research Paper

NUMERICAL SOLUTION OF SOME NON-LINEAR EIGENVALUE DIFFERENTIAL EQUATIONS BY FINITE DIFFERENCE-SELF CONSISTENT FIELD METHOD

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Abstract. The finite difference-self consistent field iteration is presented to solve some non-linear eigenvalue differential equations. Some properties of the self consistent field iteration and finite difference methods required for our subsequent development are given. Numerical examples are included to demonstrate the validity and applicability of the present technique. A comparison is also made with the existing results. The method is easy to implement and yields accurate results.

Keywords: Non-linear eigenvalue differential equation, Finite difference method, Self consistent field iteration
MSC(2010): 47j10; 35pxx.

1. Introduction

There are some papers in which non-linear eigenvalue differential equation are studied (see [5, 10]). This type of problem arises in physics, dynamic system, electronic structure calculations, etc (see [8, 11, 15]). In this paper we consider the non-linear eigenvalue differential equation

$$cY''(x) + U(x)Y'(x) + V(x)Y(x) + Q(x)Y^3(x) = EY(x), \int_a^b Y^2(x)dx = 1 \tag{1.1}$$

on (a, b), within homogeneous boundary conditions $Y(a) = Y(b) = 0$, where unknown value E and function $Y(x)$ are eigenvalues and corresponding eigenfunctions, respectively. Also $U(x)$, $V(x)$ and $Q(x)$ are known functions. For some function $V(x)$, the equation 1.1 have analytical solution [3, 4, 6]. But some other, have not exact solution and they must be solved with the numerical methods. So far different numerical methods have been used to solve Eq.1.1 by several authors, such variational method [1, 9], fixed point method [16], homotopy analysis method [2], NU method [14], etc. The present paper is devoted to the numerical solution of the Eq. 1.1 by using the finite difference-self consistent field iteration (FDSCF) method. In order to show the accuracy and robustness of the proposed schema, some examples with exact solutions are considered. This paper is organized as follows: Section 2 contains the preliminary concepts, definitions and notations of the self consistent. In Sections 3, we present the matrix of Eq. 1.1 by FDSCF method. Section 4 is devoted to the numerical

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solution of some examples by the mentioned methods. Finally, a brief conclusion is presented in Section 5.

2. Preliminaries and Notations

Let the non-linear eigenvalue problem:

$$H(X)X = \Lambda X \tag{2.1}$$

where $X \in \mathbb{R}^{n\times 1}$, $X^T X = I$, $H(X) \in \mathbb{R}^{n\times n}$ is a matrix that has a special structure and $\Lambda \in \mathbb{R}$ is a diagonal matrix consisting of the smallest eigenvalues of $H(X)$. Some researches in [12, 17] investigated the convergence of Self consistent field iteration(SCF) which defined as follow to solve problem 2.1:

(2.2)

Pick any initial guess $X^{(0)}$

1. For $i = 1, 2, ...$ until convergence
2. Construct $H^{(i)} = H(X^{(i-1)})$
3. Compute $X^{(i)}$ such that $H^{(i)}X^{(i)} = X^{(i)}\Lambda^{(i)}$ and $\Lambda^{(i)}$ contains the smallest eigenvalues of $H^{(i)}$
4. End for

Yang et al. in [17] show that for some class of problems, the SCF iteration produces a sequence of approximate solution that contain two convergent subsequence. They use of the standard distance measure [7] between tow columns $X, Y \in \mathbb{R}^{n\times k}$ i.e., if $X^T X = Y^T Y = I_k$,

$$dist(X, Y) = \|XX^T - YY^T\|_2$$

where for every matrix $A \in \mathbb{R}^{m\times n}$,

$$\|A\|_2 = \sup_{x\neq 0} \frac{\|Ax\|_2}{\|x\|_2}$$

They obtained the following theorem:

Theorem 2.1. *Let $X^{(0)} \in \mathbb{R}^{n\times k}$ be the initial guess to the solution of the non-linear eigenvalue problem 2.1 that satisfies ${X^{(0)}}^T X^{(0)} = I_k$. If columns of $X^{(i)} \in \mathbb{R}^{n\times k}$ contain eigenvectors associated with the smallest k eigenvalues of $H(X^{(i-1)})$, as we would obtain when applying the SCF iteration to problem 2.1, and if the gap between the kth and the k+1st eigenvalues of $H(X^{(i)})$ is greater than or equal to $\delta > 0$ for all i, then*

$$\lim_{i\to\infty} dist^2(Xi + 2, X_i) = 0.$$

In this paper, we obtain the matrix H by the finite difference method and use the SCF iteration to solve the problem 1.1. In continue, we present a brief overview of finite difference.

3. Main Results

In this section we obtain the matrix generated by the finite differential method. For this, let N be a positive integer, $h = \frac{b-a}{N}$ and $x_j = a + jh$ for $j = 0, ..., N$. Now by the differential method, Eq. 1.1, can be written as:

$$c\frac{Y_{j-1} + Y_{j+1} - 2Y_j}{h^2} + U_j\frac{Y_{j+1} - Y_j}{h} + V_i Y_j + Q_j|Y_j|^2 Y_j = EY_j \tag{3.1}$$

where the eigenfunction satisfies the boundary conditions $Y_0 = Y_n = 0$. Let

$$p_{j,j} = \frac{-2c}{h^2} - \frac{U_j}{h} + V_j, \quad p_{j-1,j} = p_{j-1,j} = \frac{c}{h^2} + \frac{U_j}{h} \tag{3.2}$$

for $j = 1, ..., N-1$. Then, we can write system 3.1 as

$$(X + QZ)Y = EY \tag{3.3}$$

where

$$X=\begin{bmatrix} p_{1,1} & p_{1,2} & 0 & 0 & 0 & \cdots & 0 \\ p_{2,1} & p_{2,2} & p_{2,3} & 0 & 0 & \cdots & 0 \\ 0 & p_{3,2} & p_{3,3} & p_{3,4} & 0 & \cdots & 0 \\ 0 & 0 & p_{4,3} & p_{4,4} & p_{4,5} & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \cdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & p_{n-1,n-1} \end{bmatrix}$$

$$Q=\begin{bmatrix} q_1 & 0 & \cdots & 0 \\ 0 & q_2 & & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & & q_{n-1} \end{bmatrix}$$

$$Y = \begin{bmatrix} y_1 \\ \vdots \\ y_{n-1} \end{bmatrix}$$

and $Z = (DiagY)^2$. Now we must solve the non-linear eigenvalue problem $H(Y)Y = EY$ where

$$H(Y) = X + Q(DiagY)^2 :$$

For this end, let $Z^0 = 0$. We use the following Algorithm to solve non-linear eigenvalue problem 3.3.

1. For $i = 1, 2, ...$ until convergence
2. Construct $H^{(i)} = X + QZ^{(i-1)}$
3. Compute $F^{(i)}$ such that $H^{(i)}F^{(i)} = F^{(i)}H^{(i)}$, and $E^{(i)}$ contains the smallest eigenvalues of $H^{(i)}$
4. Construct $Y^{(i)}$ such that $Y^{(i)} = \frac{F^{(i)}}{\|F^{(i)}\|}$
5. Construct $Z^{(i)} = (DiagY^{(i)})^2$
6. End for

So, we can obtain the eigenvalues and eigenfunctions of Eq. 1.1.

4. **Numerical results**

In this section, we consider Eq. 1.1 through various functions $V(x)$. We denote the eigenvalues of Eq. 1.1 with E_i. Moreover, we report the CPU time for our method. All computations were carried out using Maple software on a personal computer.

Example 4.1. Consider Eq. 1.1 on $(-1, 1)$ with $c = \frac{-1}{2}$ and $U(x) = V(x) = 0$. In [13], the eigenvalues are obtained by using the elliptic functions. Let $N = 100$ be the number of nods and $i = 10$ be the number of iterations. Table 1 and 2 represent the eigenvalues obtained from reference [13] and FDSCF for $Q(x) = -1$ and $Q(x) = -5$, respectively as well as the absolute error of FDSCF method with $Error = \|E_{Ref13} - E_{FDSCF}\|$. In figure 1, we show the convergence of this method through variation of the minimum eigenvalue as a function of the number of nodes and the number of iterations for $Q = -1$. Also, in figure 2, we show the convergence of this method through variation of the minimum eigenvalue as a function of the number of nodes and the number of iterations for $Q(x) = -5$. Figure 3, shows the convergence of this method through variation of the minimum eigenvalue as a function of Q. This figure shows that the method work better, for smaller values of the non-linear coefficient $|Q|$. We observe that the error of our method is smaller when the non-linear parameter $|Q|$ is smaller. However this is true for smaller eigenvalues. Also in figure 4, we see that for larger eigenvalues, we have not a rule of thumb???? for larger value of the eigenvalues.

Eigenvalues	FDSCF	Ref[13]	Error
E_0	0.462459047	0.462579418	0.000120371
E_1	4.442553417	4.179929550	0.262623867
E_2	10.59860958	10.35117007	0.24743951
E_3	19.21512218	18.98801387	0.22710831
E_4	30.28031329	30.091750	0.18856329
E_5	43.78267728	43.662690	0.11998728
E_6	59.70867902	59.70093840	0.00774062
E_7	78.04253889	78.20653790	0.16399901
CPU time(s)	113	-	-

TABLE 1. Comparison of eigenvalues of example 4.1 obtained by FDSCF for $Q = -1$.

Eigenvalues	FDSCF	Ref[13]	Error
E_0	-3.401183255	-3.400181294	0.001001961
E_1	2.797846407	1.049048570	1.748797837
E_2	8.746335726	7.297398975	1.448936751
E_3	17.29591993	15.95855638	1.33736355
E_4	28.33125868	27.07312364	1.25813504
E_5	41.81772984	40.64983880	1.16789104
E_6	57.73425675	56.69153305	1.04272370
E_7	76.06201420	75.19935505	0.86265915
CPU time(s)	104	-	-

TABLE 2. Comparison of eigenvalues of example 4.1 obtained by FDSCF for $Q = -5$.

Example 4.2. Consider Eq. 1.1 on $(-1, 1)$ with $c = -1$, $U(x) = 0$ and $V(x) = 0.452\cos(\pi(1-x))$. In [1], the eigenvalues are obtained by using the discretized Euler-Lagrange variational method. Let $N = 100$ and $i = 10$. Table 3 represents the smallest eigenvalue obtained from reference [1] and FDSCF method for $Q(x) = 0.5...2$. In figure 5, we show the convergence of this method through variation of the minimum eigenvalue as a function of the number of nodes and the number of iterations for $Q = 1$.

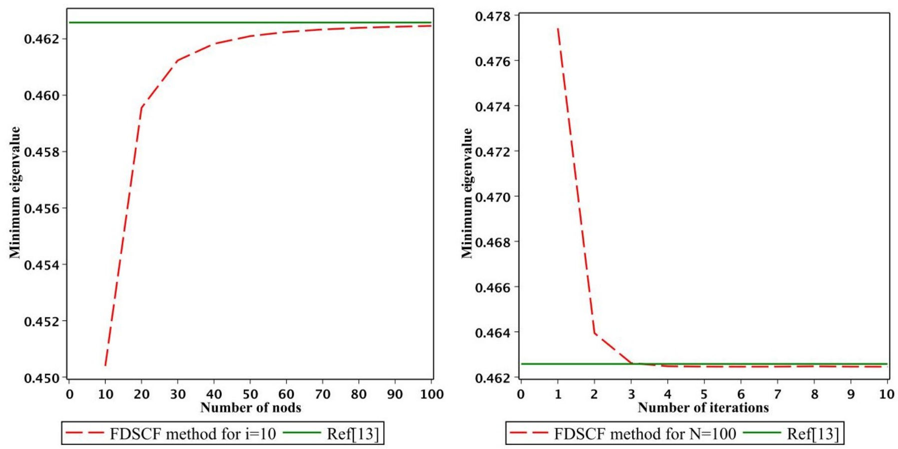

Figure 1. Left figure show the variation of the minimum eigenvalue as a function of the number of nods and right figure show the variation of the minimum eigenvalue as a function of the number of iterations for Q =-1 (example 4.1).

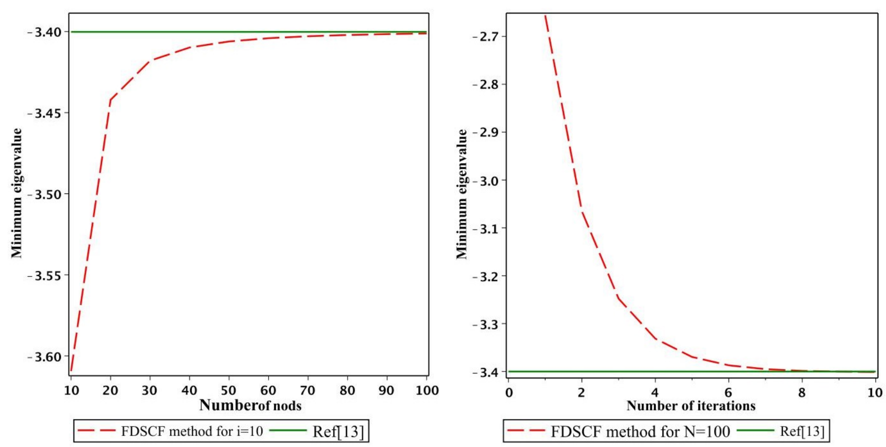

Figure 2. Left figure show the variation of the minimum eigenvalue as a function of the number of nods and right figure show the variation of the minimum eigenvalue as a function of the number of iterations for Q =-5 (example 4.1).

5. **Conclusion**

In this paper, the FDSCF method is applied to a class of non-linear eigenvalue differential equation with homogeneous boundary conditions. The eigenvalues obtained through this method are compared with exact values and some other references. To demonstrate the efficiency and effectiveness of the proposed method, two examples are examined. Based on numerical experiments, we conclude that, the method work better, for smaller values of the

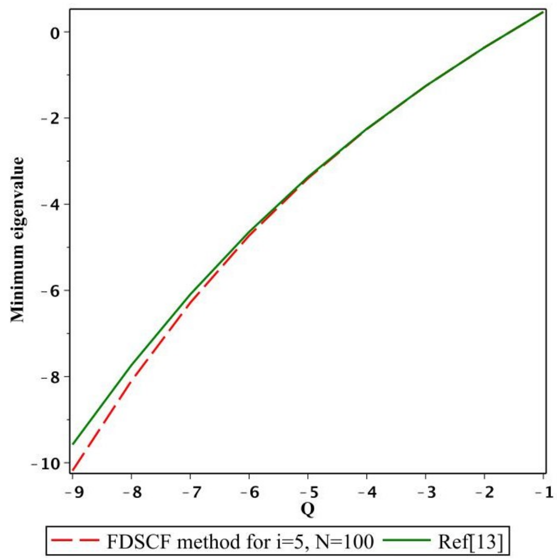

FIGURE 3. Variation of the minimum eigenvalue as a function of Q(example 4.1).

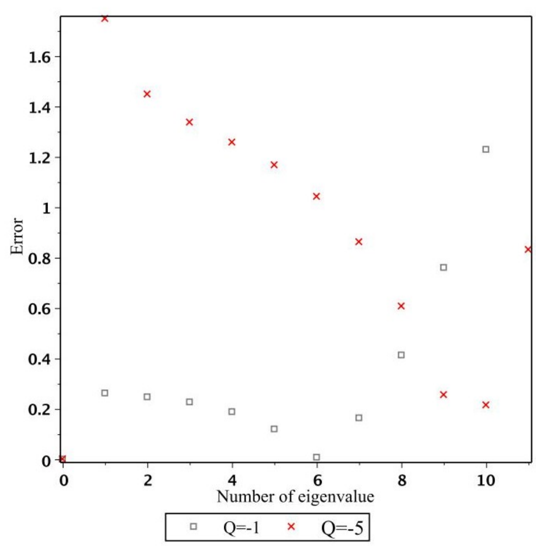

FIGURE 4. Variation of the error as a function of number of eigenvalues for Q =-1, -5(example 4.1).

non-linear coefficient $|Q|$. Also we see that the results for smallest eigenvalue have enough accuracy. But accuracy is not enough for large eigenvalues.

Q	FDSCF	Ref[1]	Error	CPU time(s)
0.5	2.616948710	2.616951848	0.3138e-05	108
1	2.990592936	2.99059549	0.2554e-05	106
1.5	3.359893114	3.35989571	0.2596e-05	112
2	3.725158240	3.725158948	0.708e-06	109

TABLE 3. Comparison of smallest eigenvalue of example 4.2 obtained by FD-SCF method.

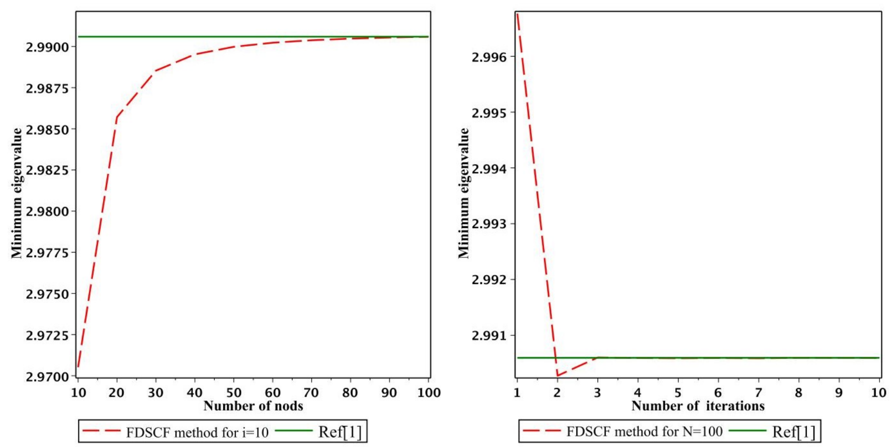

FIGURE 5. Left figure show the variation of the minimum eigenvalue as a function of the number of nods and right figure show the variation of the minimum eigenvalue as a function of the number of iterations for Q = 1 (example 4.2).

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