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

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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

\[ cY''(x) + U(x)Y'(x) + V(x)Y(x) + Q(x)Y^3(x) = EY(x), \quad \int_a^b Y^2(x)dx = 1 \]

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
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:

\[ H(X)X = \Lambda X \]

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:

\[ \text{(2.2)} \]

1. Pick any initial guess \( X^{(0)} \)
2. For \( i = 1, 2, ... \) until convergence
3. Construct \( H^{(i)} = H(X^{(i-1)}) \)
4. Compute \( X^{(i)} \) such that \( H^{(i)} X^{(i)} = X^{(i)} \Lambda^{(i)} \) and \( \Lambda^{(i)} \) contains the smallest eigenvalues of \( H^{(i)} \)
5. 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 \( X^T X = Y^T Y = I_k \),

\[ \text{dist}(X, Y) = \|XX^T - YY^T\|_2 \]

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 \( k \)th and the \( k+1 \)st eigenvalues of \( H(X^{(i)}) \) is greater than or equal to \( \delta > 0 \) for all \( i \), then

\[ \lim_{i \to \infty} \text{dist}^2(X_i + 2, X_i) = 0. \]

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:

\[ \text{(3.1)} \]

\[ c \frac{Y_{j+1} - 2Y_j + Y_{j+1}}{h^2} + U_j \frac{Y_{j+1} - Y_j}{h} + V_j Y_j + Q_j |Y_j|^2 Y_j = EY_j \]
where the eigenfunction satisfies the boundary conditions \( Y_0 = Y_n = 0 \). Let
\[
(3.2) \quad p_{j,j} = \frac{-2c}{h^2} - \frac{U_j}{h} + V_j, \quad p_{j-1,j} = p_{j,j} = \frac{c}{h^2} + \frac{U_j}{h}
\]
for \( j = 1, \ldots, N - 1 \). Then, we can write system (3.1) as
\[
(3.3) \quad (X + QZ)Y = EY
\]
where
\[
X = \begin{bmatrix}
p_{1,1} & p_{1,2} & 0 & 0 & 0 & \cdots & 0 \\
p_{2,1} & p_{2,2} & p_{2,3} & 0 & 0 & \cdots & 0 \\
0 & p_{3,2} & p_{3,3} & p_{3,4} & 0 & \cdots & 0 \\
0 & 0 & p_{4,3} & p_{4,4} & p_{4,5} & \cdots & 0 \\
\vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\
0 & 0 & 0 & 0 & 0 & \cdots & p_{n-1,n-1}
\end{bmatrix}
\]
\[
Q = \begin{bmatrix}
q_1 & 0 & \cdots & 0 \\
0 & q_2 & 0 \\
\vdots & \ddots & \ddots \\
0 & 0 & q_{n-1}
\end{bmatrix}
\]
\[
Y = \begin{bmatrix}
y_1 \\
\vdots \\
y_{n-1}
\end{bmatrix}
\]
and \( Z = (\text{Diag}Y)^2 \). Now we must solve the non-linear eigenvalue problem \( H(Y)Y = EY \) where
\[
H(Y) = X + Q(\text{Diag}Y)^2
\]
For this end, let \( Z^0 = 0 \). We use the following Algorithm to solve non-linear eigenvalue problem (3.3).
1. For \( i = 1, 2, \ldots \) 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 \( Y^{(i)} = F^{(i)}/\|F^{(i)}\| \)
5. Construct \( Z^{(i)} = (\text{Diag}Y^{(i)})^2 \)
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  | 10.3517007   | 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   |

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    |

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 \( Q(x) = 0.5 \ldots 2 \). 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.
### Table 3. Comparison of smallest eigenvalue of example 4.2 obtained by FD-SCF method.

| 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         |

**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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