BEC类非线性特征值问题的平移对称高阶幂法*

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SS-HOPM FOR BEC-LIKE NONLINEAR EIGENVALUE PROBLEMS

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Abstract We consider the nonlinear eigenvalue problem (NEP) originated from Bose-Einstein Condensation (BEC) (BEC-like NEP for short). We extend the shifted symmetric higher-order power method(SS-HOPM) proposed by Kolda and Mayo for symmetric tensor eigenvalue to BEC-like NEP. We have shown that given a proper shift term, the Algorithm SS-HOPM is convergent theorically and numerically. We also analyze the influence of data disturbance on eigenvalues theoretically and numerically.

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1 Introduction

We are concerned with a class of nonlinear eigenvalue problems over a single sphere. This problem is originated from Bose-Einstein condensates (BECs)[1-3], which recently is well known to be an important and active field[4-7] in quantum physics. Bose-Einstein condensation is that a gas of thin bosons accumulate at very low energies (or temperatures) to be a total particle in the same quantum state. The properties of a non-rotating BEC can be described by the well-known nonlinear Schrödinger equation Gross-Pitaevskii equation (GPE)[8]

$$i\hbar\frac{\partial \mathbf{u}(x,t)}{\partial t}=\left(-\frac{\hbar^2}{2m}\nabla^2+V(x)+NU_0|\mathbf{u}(x,t)|^2\right)\mathbf{u}(x,t), \tag{1.1}$$

where i is the imaginary unit, m is the atomic mass, $\hbar$ is the Planck constant, $V(x)$ is an external trapping potential, N is the number of atoms in the condensate, $U_0=\dfrac{4\pi\hbar^2a_s}{m}$ describes the interaction between atoms in the condensate(a_s denotes the s-wave scattering length).

It is convenient to normalize the wave function by requiring

$$\int_{\mathbb{R}^d}|\mathbf{u}(x,t)|^2\mathrm{d}x=1. \tag{1.2}$$

By scaling (1.1) under the normalization (1.2), we can obtain the following dimensionless GPE

$$i\frac{\partial \mathbf{u}(x,t)}{\partial t}=\left(-\frac{1}{2}\nabla^2+V(x)+\beta|\mathbf{u}(x,t)|^2\right)\mathbf{u}(x,t), \tag{1.3}$$

which governs the dynamic of the BEC, where β is the dimensionless interaction coefficient(positive for repulsive interaction and negative for attractive interaction). We just consider the stationary GPE for non-rotationg BEC. Let $\mathbf{u}(\mathbf{x},t)=\mathbf{u}(\mathbf{x})e^{-i\lambda t}$ to separate t from the

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equation. Actually, it is reasonable to assume the time and space are independent with each other in reality. Then we resort to find $\lambda \in \mathbb{R}$ and a function $\mathbf{u}$ such that

$$\begin{cases} -\frac{1}{2}\Delta \mathbf{u} + V\mathbf{u} + \beta|\mathbf{u}|^2\mathbf{u} = \lambda \mathbf{u}, \quad \text{in } \Gamma, \\ \mathbf{u} = 0, \quad \text{on } \partial\Gamma, \\ \int_\Gamma |\mathbf{u}|^2 \mathrm{d}\Gamma = 1, \end{cases} \tag{1.4}$$

where $\Gamma \subset \mathbb{R}^d (d = 1, 2, 3)$ denotes a regular bounded domain with Lipschitz boundary $\partial\Gamma$ and cone property. The energy functional in BEC problem can be defined as

$$E(\mathbf{u}) = \int_{\mathbb{R}^d} \left[\frac{1}{2}|\nabla \mathbf{u}(\mathbf{x})|^2 + V(\mathbf{x})|\mathbf{u}(\mathbf{x})|^2 + \frac{\beta}{2}|\mathbf{u}(\mathbf{x})|^4\right] \mathrm{d}\mathbf{x}. \tag{1.5}$$

The ground state of a BEC is usually defined as the global minimizer of the following nonconvex optimization problem

$$\mathbf{u}_g = \arg\min_{\mathbf{u}\in \mathbf{S}} E(\mathbf{u}) \tag{1.6}$$

where the spherical constraint $\mathbf{S}$ is defined as

$$\mathbf{S} = \left\{\mathbf{u} | E(\mathbf{u}) < \infty, \int_{\mathbb{R}^d} |\mathbf{u}(\mathbf{x})|^2 \mathrm{d}\mathbf{x} = 1\right\}. \tag{1.7}$$

From the analytical results [1], the ground state of a non-rotating BEC can be taken as a real non-negative function, while for a rotating BEC, it is always a complex function. So the nonlinear eigenvalue λ is assumed to be real. We assume that the nonlinear eigenvalue λ and its corresponding eigenfunction $\mathbf{u}$ to be real.

Actually, it can be easily verified that the nonlinear eigenvalue problem (1.4) can be viewed as the the first-order optimality condition of the energy functional $E(\mathbf{u})$ under the normalization constraint.

We can discretize the extremum problem of energy functional (1.6) with constraint (1.7) or the nonlinear eigenvalue problem (1.4) by methods such as finite difference, sine pseudospectral and Fourier pseudospectral methods. No matter which method we take to do the discretization, the discretization of the nonlinear eigenvalue problem (1.4) can be

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presented as

$$\begin{cases} \mathcal{A}\mathbf{x}^3 + \mathbf{B}\mathbf{x} = \lambda\mathbf{x} \\ ||\mathbf{x}||_2 = 1, \end{cases} \tag{1.8}$$

While the constrained minimization problem (1.6) with (1.7) can be written in tensor form as

$$\begin{aligned} \min \quad & \frac{1}{2}\mathcal{A}\mathbf{x}^4 + \mathbf{x}^\top \mathbf{B}\mathbf{x} \\ \text{s. t.} \quad & ||\mathbf{x}||_2 = 1. \end{aligned} \tag{1.9}$$

where $\mathcal{A} \in \mathbb{R}^{n\times n\times n\times n}$ is a symmetric 4th-order tensor, namely, the element of $\mathcal{A}$ may be denoted as $a_{ijkl}, i, j, k, l = 1, \cdots, n$, $\mathbf{B} \in \mathbb{R}^{n\times n}$ is a symmetric matrix, $\mathbf{x} \in \mathbb{R}^n$ is a vector. It is easy to verify that the KKT system of (1.9) is (1.8).

Nonconvex optimization problems are generally NP-hard [9]. Hu et al. [10] have shown that the BECs problem (1.9) is generally NP-hard, for it can be interpreted as a special instance of the partition problem. Actually, from the large number of variables and the possible indefinite of the Hessian matrix, one can deduce that it is a numerical challenge to solve (1.9). So the general nonlinear eigenvalue problem (1.8) is a challenge problem to solve too.

Generally, the approaches for solving BEC problem can be divided into two classes. The first calss of method is designed for the NEP (1.8) [11,12], while the second class is constructed for the minimization problem (1.9). Direct and traditional minimization approaches, such as basic gradient and trust region schemes, may still be valid for BEC problem. Actually, various gradient projection methods have been developed for solving the BEC problem. A normalized gradient flow method via the backward Euler finite difference discretization method has been extended to compute ground states of spin-1 BEC [2,13], dipolar BEC [14] and spin-orbit coupled BEC [15]. Sobolev gradient method is developed in [16,17]. A regularized Newton method is proposed in [7] by replacing the objective function with its second-order Taylor expansion and a regularization term. Recently, [10,18] established a SDP relaxation model to solve BEC with SDP(semidefinite programming)

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method. In [18], ADMM (alternating direction multiplier method) and Lasserre semidefinite programming relaxation method were established to calculate the nonlinear eigenvalues of BEC.

Kolda and Mayo [19] had proposed an algorithm to find the real-valued tensor eigenpairs of higher-order tensor. Their method is called the shifted symmetric higher-order power method (SS-HOPM), along with theoretical guarantee to converge to a stationary point of an optimization problem with sphere constraint, which can be expressed as follow.

$$\begin{aligned} \max \quad & \mathcal{A}\mathbf{x}^m \\ \text{s. t.} \quad & ||\mathbf{x}||_2 = 1, \end{aligned} \tag{1.10}$$

where $\mathcal{A}$ is assumed to be symmetric. This work has extended foundational work built by Kofidis and Regalia [20] for solving (1.10). Kofidis and Regalia have shown that the symmetric higher-order power method (S-HOPM) is not guaranteed to converge. But they provide theoretical results that under certain conditions, which almost hold in reality, the S-HOPM is convergent for even-order tensors. Kolda and Mayo generalize the results by adding a shifted term to both odd- and even-order tensors (i.e., all $m \geq 3$).

Motivated by the work of Kolda and Mayo mentioned above. We generalize the shifted symmetric higher-order power method (SS-HOPM) for the BEC-like NEP with a spherical constraint.

The main contributions of this paper are summarized as follows:

- We introduce shifted higher-order power method to compute the nonconvex optimization problem (1.9). And we give a convergence analysis of the algorithm.

- We analyze that how would the eigenvalue behave when the matrix or the tensor or both of them are perturbed by a certain level of noise.

- We give some numerical experiments about the computation of nonlinear eigenvalue and its behaviour in the disturbance of matrix.

This paper is organized as follows. Section 2 presents some preliminaries about the basic notations. In Section 3, the shifted higher-order power method for the nonconvex

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optimization problem over a single sphere is introduced. And we establish the convergence of the SS-HOPM algorithm. In section 4, we analyze the situation that when the matrix $\mathbf{B}$ or the tensor $\mathcal{A}$ are perturbed by a certain level noise matrix or tensor. In section 5, the numerical experiments are given. Conclusions are discussed in Section 6.

2 Notations and Preliminaries

Throughout the paper, we exclusively consider the tensor notation introduced in [21]. Vectors (tensors of order one) are denoted by boldface lowercase letters, e.g., $\mathbf{a}$. Matrices (tensors of order two) are denoted by boldface capital letters, e.g., $\mathbf{A}$. Higher-order tensors (order three or higher) are denoted by Euler script letters, e.g., $\mathcal{A}$. Scalars are denoted by lowercase letters, e.g., a.

A tensor is a multidimensional array. The order of a tensor is the number of dimensions. An Nth-order tensor is denoted as $\mathcal{A} \in \mathbb{R}^{I_1\times I_2\times\cdots\times I_N}$, whose $(i_1, i_2, \cdots, i_N)$ element is $a_{i_1 i_2\cdots i_N}, 1 \le i_k \le I_k, k = 1, 2, \cdots, N$. Specifically, for $N = 1$ and $N = 2$, tensors are vectors and matrices respectively. Let $\mathbb{B}$ and Σ denote the unit ball and sphere on $\mathbb{R}^n$ respectively, i. e.,

$$\mathbb{B} = \{\mathbf{x} \in \mathbb{R}^n : \|x\| \le 1\} \text{ and } \Sigma = \{\mathbf{x} \in \mathbb{R}^n : \|x\| = 1\}.$$

Definition 2.1 (Symmetry[22])) A tensor $\mathcal{A} \in \mathbb{R}^{\overbrace{n\times\cdots\times n}^{m}}$ is symmetric if

$$a_{i_{p(1)}\cdots i_{p(m)}} = a_{i_1\cdots i_m} \quad \text{for all } \ i_1\cdots i_m \in \{1, \cdots, n\} \ \text{ and } \ p \in \Pi_m.$$

where Π_m denotes the set of all permutations of $(1, \cdots, m)$.

Definition 2.2[22] (Symmetric tensor-vector multiply) Let $\mathcal{A} \in \mathbb{R}^{\overbrace{n\times\cdots\times n}^{m}}$ be symmetric and $\mathbf{x} \in \mathbb{R}^n$. Then for $0 \le r \le m-1$, the $m-r$-times product of tensor $\mathcal{A}$ with the vector $\mathbf{x}$ is denoted by $\mathcal{A}\mathbf{x}^{m-r} \in \mathbb{R}^{\overbrace{n\times\cdots\times n}^{r}}$ and defined by

$$(\mathcal{A}\mathbf{x}^{m-r})_{i_1\cdots i_r} \equiv \sum_{i_{r+1},\cdots,i_m} a_{i_1\cdots i_m} x_{r+1}\cdots x_{i_m} \quad \text{for all } \ i_1\cdots i_r \in \{1, \cdots, n\}.$$

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Definition 2.3 (Identical tensor[19,23]) If a symmetric tensor $\mathcal{E} \in \mathbb{R}^{\overbrace{n \times \cdots \times n}^{m}}$ satisfies

$$\mathcal{E}\mathbf{x}^{m-1} = \mathbf{x} \quad \text{for all} \quad \mathbf{x} \in \Sigma,$$

then $\mathcal{E}$ is called identical.

Definition 2.4[23,24] Assume that $\mathcal{A}$ is a symmetric mth-order n-dimensional real-valued tensor. If $\mathbf{x} \in \mathbb{C}^n, \lambda \in \mathbb{C}$ such that

$$\mathcal{A}\mathbf{x}^{m-1} = \lambda\mathbf{x} \quad \text{and} \quad \mathbf{x}^{\dagger}\mathbf{x} = 1, \tag{2.1}$$

then $\lambda \in \mathbb{C}$ is an eigenvalue of $\mathcal{A}$, $\mathbf{x}$ is a corresponding eigenvector, and $(\lambda, \mathbf{x})$ is called an eigenpair.

It can be verified that if $\mathbf{x}$ is real, λ is also real. Actually, if the corresponding eigenvector $\mathbf{x}$ is restricted to be real, then the λ is Z-eigenvalue defined by Qi[23] and l_2-eigenvalue defined by Lim [24]. For convenience, $\mathbf{x}$ is assumed to be real.

3 SS-HOPM for BEC-like NEP and Convergence Analysis

Higher-order power method(HOPM) [25] was a generalization of matrix power method to tensor case. It is aiming at finding the biggest singular value of a tensor. While symmetric higher-order power method(S-HOPM) [26] was extended for achieving the best rank-one approximation of a symmetric tensor. Kofidis and Regalia[20] took a further analysis on S-HOPM. They proved that the sequence $\{\lambda_k\}$ in Algorithm HOPM converges only in the condition that $f(\mathbf{x}) = \mathcal{A}\mathbf{x}^m$ being convex or concave and m being even.

Kolda and Mayo[19] developed a shifted version of the S-HOPM, called SS-HOPM, and proved that for a suitable choice of shift their algorithm will converge.

The shift α must satisfy $\alpha > \beta$ for convex case to guarantee convergence, where $\beta \equiv (m-1) \cdot \max\limits_{||\mathbf{x}||=1} \rho(\mathcal{A}\mathbf{x}^{m-2})$. While for concave case, α is required to satisfy $\alpha < -\beta$. If α is

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chosen appropriately, it can be sure that the corresponding Hessian is positive or negative definite, ensuring the objective function be locally convex or concave.

3.1 SS-HOPM for BEC-like NEP

In this section, we show that SS-HOPM can be generalized to solve

$$\begin{aligned} \min \quad & \frac{1}{2}\mathcal{A}\mathbf{x}^4 + \mathbf{x}^\top \mathbf{B}\mathbf{x} \\ \text{s. t.} \quad & ||\mathbf{x}||_2 = 1, \end{aligned} \tag{3.1}$$

where $\mathcal{A} \in \mathbb{R}^{n\times n\times n\times n}$ is a symmetric 4th-order tensor, $\mathbf{B} \in \mathbb{R}^{n\times n}$ is a symmetric matrix, $\mathbf{x} \in \mathbb{R}^n$ is a vector. Our extension is adding a suitable shift to function $f(\mathbf{x}) = \frac{1}{2}\mathcal{A}\mathbf{x}^4 + \mathbf{x}^\top\mathbf{B}\mathbf{x}$ to force

$$\hat{f}(\mathbf{x}) = f(\mathbf{x}) + \frac{1}{2}\alpha_1(\mathbf{x}^\top\mathbf{x})^2 + \alpha_2(\mathbf{x}^\top\mathbf{x}) \tag{3.2}$$

convex or concave, where $||\mathbf{x}||_2 = 1$.

We remark here that $\alpha_1(\mathbf{x}^\top\mathbf{x})^2$ is on purpose of forcing $\mathcal{A}\mathbf{x}^4$ convex (or concave), while $\alpha_2(\mathbf{x}^\top\mathbf{x})$ is to make $\mathbf{x}^\top\mathbf{B}\mathbf{x}$ convex (or concave). For simplicity, we only consider the convex case (the concave case can be treated in the same way) and assume $\mathbf{B}$ to be positive definite. So we will not consider adding $\alpha_2(\mathbf{x}^\top\mathbf{x})$ to $f(\mathbf{x})$. Because, if $\mathbf{B}$ is not positive definite, then there exists a sufficiently large $\delta > 0$ such that $\mathbf{B} + \delta\mathbf{I} \succ 0$. Then we can consider

$$\begin{aligned} \min \quad & \frac{1}{2}\mathcal{A}\mathbf{x}^4 + \mathbf{x}^\top(\mathbf{B} + \delta\mathbf{I})\mathbf{x} \\ \text{s. t.} \quad & ||\mathbf{x}||_2 = 1, \end{aligned} \tag{3.3}$$

Due to the constraint $||\mathbf{x}||_2 = 1$, the objective function in (3.3) adds only a constant to the objective function in (3.1). So the optimization problem (3.1) and (3.3) share the same optimal solution.

Remark 3.1 There are two options about the choice of δ to make sure $\mathbf{B}$ positive definite.

1. Given δ a fixed value, such that $\delta + \lambda_{\min}(\mathbf{B}) > 0$.

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2. An alternative choice is that we can increase δ gradually in a geometric progression: let $\delta_0 = 1, \delta_{i+1} = 2\delta_i,\ i = 1, \cdots$, until $\mathbf{B} + \delta_i \mathbf{I}$ is positive definite.

Based on assumption and discussion above, we need only to consider the convexity of $\mathcal{A}\mathbf{x}^4$ in (3.1), thus

$$\hat{f}(\mathbf{x}) = f(\mathbf{x}) + \frac{1}{2}\alpha(\mathbf{x}^\top \mathbf{x})^2. \tag{3.4}$$

To minimize $\hat{f}(\mathbf{x})$ on Σ is equal to minimize $f(\mathbf{x})$ plus a constant, yet the properties of the modified function force convexity and therefore lead to convergence.

Because $m = 4$ is even, the function $\hat{f}(\mathbf{x})$ in (3.4) can be interpreted as

$$\hat{f}(\mathbf{x}) = \frac{1}{2}\hat{\mathcal{A}}\mathbf{x}^4 + \mathbf{x}^\top \mathbf{B}\mathbf{x} \equiv \frac{1}{2}(\mathcal{A} + \alpha\mathcal{E})\mathbf{x}^4 + \mathbf{x}^\top \mathbf{B}\mathbf{x}$$

where $\mathcal{E}$ is the identity tensor as defined previously.

Thus, we propose method for the following problem

$$\begin{aligned} \min \quad & \frac{1}{2}(\mathcal{A} + \alpha\mathcal{E})\mathbf{x}^4 + \mathbf{x}^\top \mathbf{B}\mathbf{x} \\ \text{s. t.} \quad & ||\mathbf{x}||_2 = 1, \end{aligned} \tag{3.5}$$

where α is a constant large enough to make the objective function convex. It can be interpreted as an extension of SS-HOPM to quartic optimization problem with quadratic term. Because $\mathcal{E}\mathbf{x}^3 = \mathbf{x}$ over Σ, the nonlinear eigenvectors of

$$\begin{cases} (\mathcal{A} + \alpha\mathcal{E})\mathbf{x}^3 + \mathbf{B}\mathbf{x} = \lambda\mathbf{x} \\ ||\mathbf{x}||_2 = 1, \end{cases}$$

are the same as those of

$$\begin{cases} \mathcal{A}\mathbf{x}^3 + \mathbf{B}\mathbf{x} = \lambda\mathbf{x} \\ ||\mathbf{x}||_2 = 1, \end{cases}$$

and the eigenvalues are shifted by α.

To study the convexity of the function $f(\mathbf{x}) = \dfrac{1}{2}\mathcal{A}\mathbf{x}^4 + \mathbf{x}^\top \mathbf{B}\mathbf{x}$, and the equivalence between the constrained stationary point of function $f(\mathbf{x})$ and the corresponding eigenpairs

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of nonlinear eigenvalue problem, we need to derive the gradient and Hessian of $f(\mathbf{x})$. A similar result about the homogeneous polynomial is well known [24] and proved in [19]. For brevity, we list the results of gradient and Hessian below without proof. The proofs can be driven in the same way as in [19].

Lemma 3.2 Let $\mathcal{A} \in \mathbb{R}^{n\times n\times n\times n}$ be a symmetric tensor, and $\mathbf{B}$ be a positive definite symmetric matrix. The gradient of $f(\mathbf{x}) = \frac{1}{2}\mathcal{A}\mathbf{x}^4 + \mathbf{x}^\top\mathbf{B}\mathbf{x}$ is

$$g(\mathbf{x}) \equiv \nabla f(\mathbf{x}) = 2\mathcal{A}\mathbf{x}^3 + 2\mathbf{B}\mathbf{x} \in \mathbb{R}^n. \tag{3.6}$$

Lemma 3.3 Let $\mathcal{A} \in \mathbb{R}^{n\times n\times n\times n}$ be a symmetric tensor, and $\mathbf{B}$ be a positive definite symmetric matrix. The Hessian of $f(\mathbf{x}) = \frac{1}{2}\mathcal{A}\mathbf{x}^4 + \mathbf{x}^\top\mathbf{B}\mathbf{x}$ is

$$\mathbf{H}(\mathbf{x}) \equiv \nabla^2 f(\mathbf{x}) = 6\mathcal{A}\mathbf{x}^2 + 2\mathbf{B} \in \mathbb{R}^{n\times n}. \tag{3.7}$$

Theorem 3.4 Let $\mathcal{A} \in \mathbb{R}^{n\times n\times n\times n}$ be a symmetric tensor, and $\mathbf{B}$ be a positive definite symmetric matrix. Then $(\lambda, \mathbf{x})$ is an eigenpair of nonlinear eigenvalue problem

$$\begin{cases} \mathcal{A}\mathbf{x}^3 + \mathbf{B}\mathbf{x} = \lambda\mathbf{x} \\ ||\mathbf{x}||_2 = 1, \end{cases}$$

if and only if $\mathbf{x}$ is a constraint stationary point of minimization problem

$$\begin{aligned} \min \quad & \frac{1}{2}\mathcal{A}\mathbf{x}^4 + \mathbf{x}^T\mathbf{B}\mathbf{x} \\ \text{s. t.} \quad & \|\mathbf{x}\|_2 = 1. \end{aligned}$$

Proof As well known that [27], any constrained stationary point $\mathbf{x}_*$ of (3.1) must satisfy $\nabla f(\mathbf{x}_*) + 2\mu_*\mathbf{x}_* = 0$, i.e., $2\mathcal{A}\mathbf{x}_*^3 + 2\mathbf{B}\mathbf{x}_* + 2\mu_*\mathbf{x}_* = 0$ for some $\mu_* \in \mathbb{R}$. Thus, $\lambda_* = -\mu_*$ is the eigenvalue corresponding to $\mathbf{x}_*$. Conversely, any eigenpair meets the condition for being a constrained stationary point with $\mu_* = -\lambda_*$.

This is the connection between minimization problem and the nonlinear eigenvalue problem.

Based on the above foundation, we can express the corresponding SS-HOPM in Algorithm 1 for the nonlinear optimization problem (3.1) as bellow.

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Algorithm 1 The shifted symmetric higher-order power method (SS-HOPM)

Require:

1. Given a symmetric tensor $\mathcal{A} \in \mathbb{R}^{n\times n\times n\times n}$ and positive definite matrix $\mathbf{B}$.
2. Shift α;

Ensure:

Eigenvalue λ and the corresponding eigenvectors $\mathbf{x}$.

```
Given x_0 ∈ R^n with ||x_0||_2 = 1. Let λ_0 = A x_0^4 + x_0^T B x_0
for k = 0, 1, ··· , do
  if α ≥ 0 then
    x̂_{k+1} ← A x_k^3 + B x_k + α x_k
  else
    x̂_{k+1} ← −(A x_k^3 + B x_k + α x_k)
  end if
  x_{k+1} ← x̂_{k+1} / ||x̂_{k+1}||_2
  λ_{k+1} = A x_{k+1}^4 + x_{k+1}^T B x_{k+1}
end for
return λ = λ_{k+1}, x = x_{k+1}.
```

A large enough positive or negative shift can make sure the modified function in (3.4) convex or concave. So if α is chosen appropriately, we can ensure that the Hessian $\mathbf{H}(\mathbf{x})$ is positive or negative definite, to ensure that $\hat{f}(\mathbf{x})$ is locally convex or concave. In Algorithm 1, the α needs to be given to ensure the convexity on the entire sphere. However, it is challenging to choose a reasonable value in advance. Because poor choices may lead to either slow convergence or lack of convergence. We leave that how to choose α properly as a topic for our future study.

3.2 Convergence analysis on SS-HOPM for BEC-like NEP

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We establish a few key lemmas to guide the choice of the shift α and to benefit the analysis on convergence.

Lemma 3.5[28] If $\mathbf{D}, \mathbf{E}$ are n-by-n symmetric matrices, then

$$\lambda_k(\mathbf{D}) + \lambda_n(\mathbf{E}) \leq \lambda_k(\mathbf{D}+\mathbf{E}) \leq \lambda_k(\mathbf{D}) + \lambda_1(\mathbf{E}), \quad k = 1, \cdots, n$$

where λ_k denote the k-th largest eigenvalue of the matrices.

As is well known to all that a symmetric matrix is positive definite is equivalent to that its smallest eigenvalue is positive. So if we need $\mathbf{D}+\mathbf{E}$ to be positive definite, then we need only that $\lambda_n(\mathbf{D}+\mathbf{E})$ is positive. From the above theorem, we know that $\lambda_n(\mathbf{D}) + \lambda_n(\mathbf{E}) \leq \lambda_n(\mathbf{D}+\mathbf{E})$, so if we can guarantee that $\lambda_n(\mathbf{D}) + \lambda_n(\mathbf{E})$ is positive, then $\mathbf{D}+\mathbf{E}$ must be positive definite.

In order to deduce the shifted term α, we define a parameter β as follow.

Definition 3.6 Let $\mathcal{A} \in \mathbb{R}^{n\times n\times n\times n}$ be a symmetric tensor, $\mathbf{B}$ be a positive definite symmetric matrix. Define

$$\beta \equiv \max_{\mathbf{x}\in\Sigma} \rho(3\mathcal{A}\mathbf{x}^2 + \mathbf{B}). \tag{3.8}$$

Lemma 3.7 Let $\mathcal{A} \in \mathbb{R}^{n\times n\times n\times n}$ be a symmetric tensor, $\mathbf{B}$ be a positive definite symmetric matrix, $f(\mathbf{x}) = \dfrac{1}{2}\mathcal{A}\mathbf{x}^4 + \mathbf{x}^\top\mathbf{B}\mathbf{x}$, $\mathbf{H}(\mathbf{x}) \equiv \nabla^2 f(\mathbf{x}) = 6\mathcal{A}\mathbf{x}^2 + 2\mathbf{B}$ and β is defined as in (3.8). Then

(a) β is bounded above;

(b) $f(\mathbf{x})$ is bounded for all $\mathbf{x} \in \Sigma$;

(c) The spectrum of $\mathbf{H}(\mathbf{x})$ satisfy $\rho(H(\mathbf{x})) \leq 6\rho(\mathcal{A}\mathbf{x}^2) + 2\rho(\mathbf{B})$ for all $\mathbf{x} \in \Sigma$.

Proof (a) For all $\mathbf{x}, \mathbf{y} \in \Sigma$, we apply the triangle inequality to $\mathcal{A}\mathbf{x}^2$ and $\mathbf{B}$ respectively. Then we can obtain $\left|\mathbf{y}^T\left(\mathcal{A}\mathbf{x}^2\right)\mathbf{y}\right| \leq \sum\limits_{i_1,\ldots,i_4} |a_{i_1\ldots i_4}|$ and $\left|\mathbf{y}^T\mathbf{B}\mathbf{y}\right| \leq \sum\limits_{i_1 i_2} |b_{i_1 i_2}|$. By applying Lemma 3.5 and triangle inequality, we have $\rho(3\mathcal{A}\mathbf{x}^2 + \mathbf{B}) \leq 3\rho(\mathcal{A}\mathbf{x}^2) + \rho(\mathbf{B})$. Then β is bounded above.

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(b)

$$
\begin{aligned}
|f(\mathbf{x})| &= \left|\frac{1}{2}\mathcal{A}\mathbf{x}^4+\mathbf{x}^\top\mathbf{B}\mathbf{x}\right| = \left|\mathbf{x}^\top\left(\frac{1}{2}\mathcal{A}\mathbf{x}^2+\mathbf{B}\right)\mathbf{x}\right| \\
&= \left|\mathbf{x}^\top\frac{1}{6}\left(3\mathcal{A}\mathbf{x}^2+\mathbf{B}\right)\mathbf{x}+\mathbf{x}^\top\left(\frac{5}{6}\mathbf{B}\right)\mathbf{x}\right| \\
&\le \frac{1}{6}\rho\left(3\mathcal{A}\mathbf{x}^2+\mathbf{B}\right)+\frac{5}{6}\rho(\mathbf{B}) \\
&\le \beta/6+5\rho(\mathbf{B})/6.
\end{aligned}
$$

So $f(\mathbf{x})$ is bounded for all $\mathbf{x}\in\Sigma$.

(c) The proof is obvious from the definition of β and the triangle inequality.

Theorem 3.8[20] Let f be a function that is convex and continuously differentiable on $\mathbb{B}$. If $\mathbf{v},\mathbf{w}\in\Sigma$ with $\nabla f(\mathbf{w})/\|\nabla f(\mathbf{w})\|\neq\mathbf{w}$, then $f(\mathbf{v})-f(\mathbf{w})>0$.

Based on the above lemmas and theorem, we can induce the convergence of Algorithm 1, which is similar with the Theorem 4.4 in [19]. And the proof can be similarly carried on easily, so is omitted. We present the theorem as below.

Theorem 3.9 Let $\mathcal{A}\in\mathbb{R}^{n\times n\times n\times n}$ be a symmetric tensor, $\mathbf{B}$ be a positive definite symmetric matrix. For $\alpha>\beta$, where β is defined in (3.8). The iterates $\{\lambda_k,\mathbf{x}_k\}$ generated by Algorithm 1 satisfy the following properties.

(a) The sequence $\{\mathbf{x}_k\}$ has an accumulation point $\mathbf{x}_*$.

(b) The sequence $\{\lambda_k\}$ is nondecreasing, and there exists λ_* such that $\lambda_k\to\lambda_*$, where $\lambda_k=\mathcal{A}\mathbf{x}_k^4+\mathbf{x}_k^\top\mathbf{B}\mathbf{x}_k$ and $\lambda_*=\mathcal{A}\mathbf{x}_*^4+\mathbf{x}_*^\top\mathbf{B}\mathbf{x}_*$.

(c) For each such accumulation point $\mathbf{x}_*$, the pair $(\lambda_*,\mathbf{x}_*)$ is an eigenpair of NEP (1.8).

(d) If (1.8) has finitely many real eigenpairs, then there exists $\mathbf{x}_*$ such that $\mathbf{x}_k\to\mathbf{x}_*$.

As for the concave case, a similar corollary can be obtained.

4 Perturbation Analysis on BEC-like NEP and BEC Problem

In practice, data can not avoid to be disturbed in general. In NEP (1.8), the core data is the tensor $\mathcal{A}$ and the matrix $\mathbf{B}$. The probable noise may be in the tensor $\mathcal{A}$ or the matrix

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$\mathbf{B}$, or both of them. For more details of the general BEC-like NEP, we need to consider that how would the λ perform when tensor and matrix are perturbed.

We divide the noise into two kinds, i.e., the regular noise and the random noise. We name a regular perturbation to matrix $\mathbf{B}$ as $\epsilon\mathbf{B}$, where ϵ is a little constant. Usually, ϵ is assumed to be in $[-0.05, 0.05]$. When $\epsilon > 0$, we say that matrix $\mathbf{B}$ has a positive perturbation; when $\epsilon < 0$, we say that matrix $\mathbf{B}$ has a negative perturbation. For tensor $\mathcal{A}$ we have the same notions.

For brevity, we consider that $\mathcal{A}$ and $\mathbf{B}$ in general BEC-like NEP are disturbed by $\delta\mathcal{A}, \delta\mathbf{B}$ at the same time while not dividing into several cases, thus

$$\begin{cases} (\mathcal{A}+\delta\mathcal{A})\mathbf{x}^3 + (\mathbf{B}+\delta\mathbf{B})\mathbf{x} = \lambda\mathbf{x} \\ ||\mathbf{x}||_2 = 1. \end{cases}$$

where, $\delta\mathcal{A}, \delta\mathbf{B}$ are noise to $\mathcal{A}$ and $\mathbf{B}$.

In order to study the behaviour of the eigenvalue λ in the perturbation of matrix and tensor, we have to make some assumptions. First, the noise, no matter regular or random, is given. Second, to keep consistent with the original problem, we assume that the noise is symmetric in the sense of tensor or matrix.

Define $\lambda_O \equiv \max\{\mathcal{A}\mathbf{x}^4 + \mathbf{x}^\top\mathbf{B}\mathbf{x} |\ ||\mathbf{x}||_2 = 1\}$ and $\lambda_p \equiv \max\{(\mathcal{A}+\delta\mathcal{A})\mathbf{x}_p^4 + \mathbf{x}_p^\top(\mathbf{B}+\delta\mathbf{B})\mathbf{x}_p |\ ||\mathbf{x}_p||_2 = 1\}$, where $\mathbf{x}_p$ is the corresponding eigenvector to λ_p. Now what we want to know is the relation among the $\lambda_O, \lambda_p, \delta\mathcal{A}$ and $\delta\mathbf{B}$.

We utilize the form in [10] to transform our problem into a homogeneous form as

$$\begin{cases} \lambda_O \equiv \mathcal{A}\mathbf{x}^4 + \mathbf{x}^\top\mathbf{x}\mathbf{x}^\top\mathbf{B}\mathbf{x} = (\mathcal{A} + \mathrm{sym}(\mathbf{B}\circ I))\mathbf{x}^4 \\ ||\mathbf{x}||_2 = 1. \end{cases}$$

and

$$\begin{cases} \lambda_p \equiv (\mathcal{A}+\delta\mathcal{A})\mathbf{x}_p^4 + \mathbf{x}_p^\top\mathbf{x}_p\mathbf{x}_p^\top(\mathbf{B}+\delta\mathbf{B})\mathbf{x}_p = (\mathcal{A}+\delta\mathcal{A} + \mathrm{sym}((\mathbf{B}+\delta\mathbf{B})\circ I))\mathbf{x}^4 \\ ||\mathbf{x}_p||_2 = 1. \end{cases}$$

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The symbol "$\circ$" represents the matrix outer product. Next, we transform the above two formulations into tensor forms

$$\lambda_O \equiv \max\{\mathcal{F}\mathbf{x}^4 \mid \|\mathbf{x}\|_2 = 1.\} \quad \text{and} \quad \lambda_p \equiv \max\{\hat{\mathcal{F}}\mathbf{x}_p^4 \mid \|\mathbf{x}_p\|_2 = 1.\}$$

where $\mathcal{F} = \mathcal{A} + \mathrm{sym}(\mathbf{B} \circ \mathbf{I}), \hat{\mathcal{F}} = \mathcal{A} + \delta\mathcal{A} + \mathrm{sym}((\mathbf{B} + \delta\mathbf{B}) \circ \mathbf{I})$ are symmetric tensors, and they can be expressed as the following forms respectively,

$$\mathcal{F}_{\pi(i,j,k,l)} = \begin{cases} b_{kl}/2 + a_{ijkl}, & i = j = k \neq l \\ b_{kl}/6 + a_{ijkl}, & i = j, \quad i \neq k, \quad i \neq l, \quad k \neq l \\ (b_{ii} + b_{kk})/6 + a_{ijkl}, & i = j \neq k = l \\ b_{ii} + a_{ijkl}, & i = j = k = l \\ 0, & \text{otherwise} \end{cases}$$

$$\hat{\mathcal{F}}_{\pi(i,j,k,l)} = \begin{cases} \dfrac{b_{kl} + \delta b_{kl}}{2} + (a_{ijkl} + \delta a_{ijkl}), & i = j = k \neq l \\ (b_{kl} + \delta b_{kl})/6 + (a_{ijkl} + \delta a_{ijkl}), & i = j, \quad i \neq k, \quad i \neq l, \quad k \neq l \\ (b_{ii} + b_{kk} + \delta b_{ii} + \delta b_{kk})/6 + (a_{ijkl} + \delta a_{ijkl}), & i = j \neq k = l \\ b_{ii} + \delta b_{ii} + (a_{ijkl} + \delta a_{ijkl}), & i = j = k = l \\ 0, & \text{otherwise} \end{cases}$$

Based on the discussion above, we can deduce that $\hat{\mathcal{F}} = \mathcal{F} + \delta\mathcal{F}$, where $\delta\mathcal{F} = \delta\mathcal{A} + \mathrm{sym}(\delta\mathbf{B} \circ \mathbf{I})$. While $\mathrm{sym}(\delta\mathbf{B} \circ I)$ is symmetric form of the tensor $\delta\mathbf{B} \circ \mathbf{I}$. We can describe λ_O and λ_p in a succinct form and deduce the error to the original eigenvalue.

$$\frac{\|\lambda_p - \lambda_O\|}{\|\lambda_O\|} = \frac{\|\hat{\mathcal{F}}\mathbf{x}_p^4 - \mathcal{F}\mathbf{x}^4\|}{\|\mathcal{F}\mathbf{x}^4\|} = \frac{\|(\mathcal{F} + \delta\mathcal{F})\mathbf{x}_p^4 - \mathcal{F}\mathbf{x}^4\|}{\|\mathcal{F}\mathbf{x}^4\|} = \frac{\|\mathcal{F}\mathbf{x}_p^4 - \mathcal{F}\mathbf{x}^4 + \delta\mathcal{F}\mathbf{x}_p^4\|}{\|\mathcal{F}\mathbf{x}^4\|}$$

Since $\mathbf{x}, \mathbf{x}_p$ are the corresponding eigenvectors to largest Z-eigenvalue λ_O, λ_p of tensor $\mathcal{F}, \hat{\mathcal{F}}$. Then we must have $\mathcal{F}\mathbf{x}_p^4 \leq \mathcal{F}\mathbf{x}^4$ and $(\mathcal{F} + \delta\mathcal{F})\mathbf{x}_p^4 \geq (\mathcal{F} + \delta\mathcal{F})\mathbf{x}^4$. Then no matter the disturbance increase or decrease the eigenvalue, we can assure that

$$\delta\mathcal{F}\mathbf{x}_p^4 \geq \lambda_p - \lambda_O \geq \delta\mathcal{F}\mathbf{x}^4.$$

So

$$\|\lambda_p - \lambda_O\| \leq \max\{\|\delta\mathcal{F}\mathbf{x}^4\|, \|\delta\mathcal{F}\mathbf{x}_p\|^4\}.$$

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Then

$$\frac{\|\lambda_p - \lambda_O\|}{\|\lambda_O\|} \le \max\left\{\frac{\|\delta\mathcal{F}\mathbf{x}^4\|}{\|\mathcal{F}\mathbf{x}^4\|}, \frac{\|\delta\mathcal{F}\mathbf{x}_p^4\|}{\|\mathcal{F}\mathbf{x}^4\|}\right\}.$$

In order to simplify the expression, we relax the right two terms in the brace of the inequality above. We assume that $\hat{\mathbf{x}}$ is the eigenvector corresponding to the spectrum eigenvalue of $\delta\mathcal{F}$, noted as $\rho(\delta\mathcal{F})$. So we have $\|\delta\mathcal{F}\mathbf{x}^4\| \le \|\rho(\delta\mathcal{F})\|$ and $\|\delta\mathcal{F}\mathbf{x}_p^4\| \le \|\rho(\delta\mathcal{F})\|$. Thus we achieve that

$$\frac{\|\lambda_p - \lambda_O\|}{\|\lambda_O\|} \le \frac{\|\rho(\delta\mathcal{F})\|}{\|\lambda_O\|}. \tag{4.1}$$

Actually, the spectrum $\rho(\delta\mathcal{F})$ can be defined as the maximum of the absolute value of eigenvalue $\delta\mathcal{F}$.

For the perturbation to the minimum eigenvalue of $\mathcal{F}$, we can do the similar deduction as above. We just list the final result as bellow

$$\frac{\|\lambda_p - \lambda_O\|}{\|\lambda_O\|} \le \frac{\|\rho(\delta\mathcal{F})\|}{\|\lambda_O\|}. \tag{4.2}$$

Although the two formulas (4.1) and (4.2) are formally identical, we must note that each parameter represents a different meaning, except that $\rho(\delta\mathcal{F})$.

Back to the perturbation of our original problem, we can obtain the concise formula for each kind of noise to the general BEC-like NEP.

1. If the noise is happening only to the matrix $\mathbf{B}$, thus $\|\rho(\delta\mathcal{F})\| = \|\rho(\mathrm{sym}(\delta\mathbf{B} \circ \mathbf{I}))\|$.

2. If the noise is happening only to the tensor $\mathcal{A}$, thus $\|\rho(\delta\mathcal{F})\| = \|\rho(\delta\mathcal{A})\|$.

3. If noise have influence both of the matrix and tensor, then $\|\rho(\delta\mathcal{F})\| = \|\rho(\delta\mathcal{A} + \mathrm{sym}(\delta\mathbf{B} \circ \mathbf{I}))\|$.

5 Numerical Examples

In this section, we report some numerical examples to illustrate the accuracy and efficiency of SS-HOPM scheme proposed in this paper. All experiments were performed on a PC with 1.8GHz CPU (i5 Core) and 8G ROM, and algorithm is implemented in MATLAB (R2015b) and Tensor Toolbox [29]. In our experiments, we want to utilize Algorithms

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SS-HOPM to compute the maximum or the minimum nonlinear eigenvalue of a general BEC-like NEP and BEC problem. The algorithm stops either when a maximal number of K iterations is reached or when

$$\left\|\mathcal{A}\mathbf{x}_k^3+\mathbf{B}\mathbf{x}_k-\lambda_k\mathbf{x}_k\right\|_\infty<\varepsilon_0 \tag{5.1}$$

The default values of ε_0 and K are set to be 10^{-12} and 100000 for BEC-like NEPs, respectively. Because the computation scale maybe enlarge by the density of $\mathcal{A}$ and $\mathbf{B}$. While in BEC problem, we set ε_0 and K to be 10^{-12} and 1000000, respectively. Since we know $\mathcal{A}$ and $\mathbf{B}$ are sparse, that may reduce the computation burden. We remark here that the error may have some other options, for example, $|f(\mathbf{x}_{k+1})-f(\mathbf{x}_k)|$, $|\lambda_k-\lambda_{k+1}|$ or $\|\mathbf{x}_{k+1}-\mathbf{x}_k\|_\infty$.

5.1 Numerical results for general BEC-like NEPs

Take $\mathcal{A}\in\mathbb{R}^{n\times n\times n\times n}$ to be a symmetric tensor, $\mathbf{B}\in\mathbb{R}^{n\times n}$ to be a positive definite symmetric matrix. We show results using Algorithm SS-HOPM to compute the maximum or minimum of (1.8). We consider $n=10,20,30,40,50$ respectively. The tensor $\mathcal{A}$, matrix $\mathbf{B}$ and the initial vector $\mathbf{x}_0$ are generated randomly in each scale at first, and we store them for further test. Tables depict the numerical results of the nonlinear eigenvalue λ, error, iterations and CPU time for the Algorithm SS-HOPM in different scale n.

Table 1 General BEC-like NEP with SS-HOPM

n	maximum				minimum			
	λ	error	iteration	time(s)	λ	error	iteration	time(s)
10	19.1554	9.46e-13	370	1.163758	-11.5956	9.59e-13	329	1.032451
20	31.7124	9.34e-13	599	2.962184	-28.7891	9.14e-13	328	1.589947
30	42.6003	9.51e-13	402	4.299910	-34.6680	9.73e-13	717	7.638428
40	43.3803	9.97e-13	1279	31.814492	-43.2741	9.90e-13	1390	32.321997
50	49.3916	9.89e-13	2033	117.143496	-53.8764	9.78e-13	949	54.350721

The Algorithm SS-HOPM is stable for our problem. It converges to a local optimum. Actually, we can expect they converge to a global optimum if we test enough from different

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starting points. But in reality, we can not assure that the result is the optimal. We have tested the BEC-like NEP with fixed $\mathcal{A}$ and $\mathbf{B}$ that starting from different initial $\mathbf{x}_0$, we may obtain better λ. So we may not gain the global but local maximum or minimum with the algorithm. Thus, how to pick up a good initial value may be a question of worthy of study.

Remark 5.1

1. The SS-HOPM is a economical and stable method for our problem.

2. For SS-HOPM, sequence $\{\lambda_k\}$ is always either a nondecreasing or nonincreasing sequence for the nonlinear eigenvalue problem.

3. The initial choice of $\mathbf{x}_0$ has a great influence on the iteration time and number, even the result.

5.2 Numerical results for BEC problem

We consider the succinct form of BEC problem as follow

$$\begin{cases} -\Delta\mathbf{u}(\mathbf{x}) + V(\mathbf{x})\mathbf{u} + \xi|\mathbf{u}(\mathbf{x})|^2\mathbf{u}(\mathbf{x}) = \lambda\mathbf{u}(\mathbf{x}), \quad \text{in } \Gamma, \\ \mathbf{u}(\mathbf{x}) = 0, \quad \text{on } \partial\Gamma, \\ \int_\Gamma |\mathbf{u}(\mathbf{x})|^2 \mathrm{d}\Gamma = 1, \end{cases}$$

where $\Gamma = [0,1]^d$ denotes the solving domain, $d = 1,2,3$ is the dimension of domain. Thus we have three cases, i.e. BEC in one, two and three dimension. Let $\xi = 1$ for simplicity. We consider the harmonic potential

$$V(\mathbf{x}) = \begin{cases} \gamma_x^2 x^2, \quad d = 1, \\ \gamma_x^2 x^2 + \gamma_y^2 y^2, \quad d = 2, \\ \gamma_x^2 x^2 + \gamma_y^2 y^2 + +\gamma_z^2 z^2, \quad d = 3, \end{cases}$$

where $\gamma_x, \gamma_y, \gamma_y$ are three given positive constants, and we let them all to be 1.

First, we consider $\Gamma = [0,1]$. If we divide Γ in n equally and discrete the boundary value problem by finite difference scheme, then we can obtain a nonlinear eigenvalue problem as

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follow

$$\begin{cases} \mathcal{A}\mathbf{x}^3 + \mathbf{B}\mathbf{x} = \lambda\mathbf{x} \\ ||\mathbf{x}||_2^2 = n, \end{cases} \tag{5.2}$$

where $\mathcal{A}$ is an order-4, $n-1$-dimension diagonal one tensor, $\mathbf{x} = (x_1, x_2, \cdots, x_{n-1})^\top$, $\mathcal{A}\mathbf{x}^3 = (x_1^3, x_2^3, \cdots, x_{n-1}^3)^\top$, and $\mathbf{B}$ is a tridiagonal matrix as follow

$$\mathbf{B} = n^2 \begin{pmatrix} 2 & -1 & & \\ -1 & 2 & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 2 \end{pmatrix} + \frac{1}{n^2} \begin{pmatrix} 1 & & & \\ & 4 & & \\ & & \ddots & \\ & & & (n-1)^2 \end{pmatrix}.$$

We can gain similar nonlinear eigenvalue problem as (5.2) in two and three dimension. Thus, if we divide the domain into n evenly in each direction, then $\mathbf{x}$ is of $(n-1)^2$ and $(n-1)^3$ dimension respectively. And the constriction surfaces become $||\mathbf{x}||_2^2 = n^2$ and $||\mathbf{x}||_2^2 = n^3$ respectively. In the three scenarios, the matrix $\mathbf{B}$ is diagonally dominant with nonpositive off-diagonal elements and it is positive definite.

In reality, we do care about the least eigenvalue of BEC, for it denotes the energy of ground state of BEC, which is in a steady state. While other eigenvalue represent the energies of various excited states, which are in quantum instability. We hope we can approximate the maximum eigenvalue of BEC by subdividing the region continuously. However, from the data in Table 2, we can see that, the maximum λ is multiplying, that is actually consistent with the scale of our problem. We may conclude that we can not gain the maximum through this kind of discretization, although we know that the greatest eigenvalue does exist, since $\lambda = \mathcal{A}\mathbf{x}^4 + \mathbf{x}^\top\mathbf{B}\mathbf{x}$ is a continuous function on a compact set Σ.

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Table 2 BEC problem(maximum)-1D case with SS-HOPM

value	n=10	n=20	n=50	n =100	n =200	n =500
λ	392.0047	1591.9435	9991.9262	39991.9238	159991.9224	999991.8459
error	1.32e-8	1.72e-8	4.55e-9	9.02e-8	2.90e-7	1.91e-6
iteration	142	664	2600	8269	38466	112553
CPU time(s)	0.005947	0.021144	0.112762	0.442765	3.3.708579	17.260627

It is more meaningful to study the ground state of BEC, so for the three cases, we only do computation for the least eigenvalue now. We have done a series experiments in different initial $\mathbf{x}_0$. We just list a few of them to claim our observations by form of tables.

Table 3 BEC problem(minimum)-1D case with SS-HOPM

value	n=10	n=20	n=50	n=100	n=200	n=500
λ	11.5612	11.6225	11.6396	11.6421	11.6429	11.6429
error	1.32e-8	1.43e-8	3.40-9	4.59e-8	6.00e-9	2.35e-7
iteration	65	160	1038	2947	7260	25333
CPU time(s)	0.024265	0.026261	0.053422	0.191161	0.685535	3.036920

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Table 4 BEC problem(minimum)-2D case with SS-HOPM

value	n=10	n=20	n=30	n=40	n=50	n=100
λ	22.3486	22.4724	22.4953	22.5034	22.5071	22.5121
error	7.222e-10	3.10e-9	7.11e-9	7.12e-9	2.00e-8	7.99e-8
iteration	579	2252	4952	7922	12923	50092
CPU time(s)	0.062822	0.424424	2.565217	16.898139	67.758191	4214.997845

Table 5 BEC problem(minimum)-3D case with SS-HOPM

value	n=5	n=10	n=15	n=20	n=25	n=30
λ	32.6881	33.4450	33.5856	33.6348	33.6576	33.6700
error	2.04e-10	1.11e-9	1.00e-9	4.67e-9	7.37e-9	1.06e-8
iteration	214	838	1893	3335	4955	7319
CPU time(s)	0.027396	0.371216	13.016069	123.192180	838.793852	3556.917216

From Tables 3-5, we can see that minimum λ is increasing with n. These provide us a numerical certification of the convergence of Algorithm SS-HOPM. For the one dimension case, when n is more than 200, the eigenvalue λ remains unchanged at 11.6429. While for the other two cases, we have not gain an unchanged value with n, since that in two or three dimension case we can just calculate the λ in a small scale n for the size of the problem here increases with n squared or cubic. We leave that how to calculate λ in a much bigger scale as a future topic.

Remark 5.2

1. The initial choice of $\mathbf{x}_0$ has influence on the iteration time and number for the BEC problem, but makes no difference to the result.

2. The SS-HOPM algorithm performs excellent in small scale n, but in a much bigger scale n it is in lack of efficiency.

3. For BEC problem, we do care the ground state, in which the minimum eigenvalue

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denote the smallest energy. The ground state is stable, while the excited state is unstable, which we can see from that the maximum eigenvalue is increasing with scale and the minimum eigenvalue is convergent with the n increasing.

5.3 Performance of λ with perturbation to matrix

We only consider that how would the λ perform numerically when the matrix is perturbed in this subsection. As for the BEC problem, tensor $\mathcal{A}$ in BEC problem is originated from Planck constant, so it is reasonable that we assume it can not be perturbed. So for BEC-like NEP, we only consider the matrix perturbation. First, we would add regular perturbation to matrix, and see what will happen to λ. Second, we will find out the change of λ with a random perturbation to matrix. We remark here that we do all the tests by SS-HOPM algorithm.

5.3.1 Regular perturbation to matrix B

Let the regular perturbation to matrix $\mathbf{B}$ be $\epsilon\mathbf{B}$, where $\epsilon \in [-0.05, 0.05]$. We have done a series of trials on various matrix scale with different ϵ for the two cases. Some of the results are listed as bellow. More over, for better comparison, we utilize the data $\mathcal{A}, \mathbf{B}, \mathbf{x}_0$ stored previously in the following experiments for BEC-like NEP.

Table 6 matrix **B** in BEC problem (1D) is regularly perturbed

n	$\epsilon=0$	$\epsilon=-0.05$	$\epsilon=-0.03$	$\epsilon=-0.01$	$\epsilon=0.01$	$\epsilon=0.03$	$\epsilon=0.05$
10	11.5612	11.0572	11.2588	11.4604	11.6620	11.8636	12.0652
20	11.6225	11.1154	11.3182	11.5211	11.7239	11.9267	12.1294
50	11.6396	11.1318	11.3349	11.5381	11.7422	11.9443	12.1475
100	11.6421	11.1341	11.3373	11.5405	11.7437	11.9469	12.1500
200	11.6429	11.1347	11.3379	11.5411	11.7443	11.9475	12.1507
500	11.6429	11.1348	11.3381	11.5413	11.7445	11.9477	12.1509

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Table 7 matrix **B** in BEC problem (2D) is regularly perturbed

n	$\epsilon=0$	$\epsilon=-0.05$	$\epsilon=-0.03$	$\epsilon=-0.01$	$\epsilon=0.01$	$\epsilon=0.03$	$\epsilon=0.05$
10	22.3486	21.3393	21.7431	22.1468	22.5504	22.9504	23.3576
20	22.4724	21.4572	21.8633	22.2694	22.6754	23.0816	23.4874
30	22.4953	21.4790	21.8856	22.2921	22.6986	23.1050	23.5112
40	22.5034	21.4867	21.8934	22.3001	22.7067	23.1133	23.5199
50	22.5071	21.4902	21.8970	22.3038	22.7105	23.1171	23.5238

Table 8 matrix **B** in BEC problem (3D) is regularly perturbed

n	$\epsilon=0$	$\epsilon=-0.05$	$\epsilon=-0.03$	$\epsilon=-0.01$	$\epsilon=0.01$	$\epsilon=0.03$	$\epsilon=0.05$
n=5	32.6881	31.2053	31.7985	32.3916	32.9846	33.5775	34.1703
n=10	33.4450	32.9276	32.5346	33.1416	33.7484	34.3552	34.9619
n=15	33.5856	32.0616	32.6713	33.2808	33.8903	34.4996	35.1089
n=20	33.6348	32.1086	32.7191	33.3296	33.9400	34.5502	35.1604

Table 9 matrix **B** in BEC-like NEP is regularly perturbed(maximum)

n	$\epsilon=0$	$\epsilon=-0.05$	$\epsilon=-0.03$	$\epsilon=-0.01$	$\epsilon=0.01$	$\epsilon=0.03$	$\epsilon=0.05$
10	19.1554	19.1347	19.1430	19.1513	19.1595	19.1678	19.1760
20	31.7124	31.6788	31.6922	31.7057	31.7191	31.7325	31.7460
30	42.6003	42.5671	42.5804	42.5937	42.6069	42.6202	42.6335
40	43.3803	43.3630	43.3669	43.3768	43.3837	43.3907	43.3976
50	49.3916	49.3739	49.3810	49.3881	49.3951	49.4022	49.4093

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Table 10 matrix **B** in BEC-like NEP is regularly perturbed(minimum)

n	$\epsilon=0$	$\epsilon=-0.05$	$\epsilon=-0.03$	$\epsilon=-0.01$	$\epsilon=0.01$	$\epsilon=0.03$	$\epsilon=0.05$
10	-11.5956	-11.6166	-11.6082	-11.5998	-11.5914	-11.5830	-11.5747
20	-28.7891	-28.8229	-28.8094	-28.7958	-28.7823	-28.7688	-28.7552
30	-34.6680	-34.69033	-34.6814	-34.6725	-34.6636	-34.6546	-34.6457
40	-43.2741	-43.2910	-43.2843	-43.2775	-43.2707	-43.2639	-43.2572
50	-53.8764	-53.8998	-53.8904	-53.8811	-53.8717	-53.8624	-53.8530

From Tables 6 to 10, we can find out a co-directional change between eigenvalues and perturbations, i.e., the eigenvalue λ of both cases change in the same direction of perturbation. From perturbation analysis, we have

$$\frac{\|\rho(\delta\mathcal{F})\|}{\|\lambda_O\|} \leq \frac{\|\rho(\delta\mathbf{B})\|}{\|\rho(\mathbf{B})\|} = \epsilon.$$

We can easily verify that the relative errors of eigenvalue induced by matrix perturbation in one dimension BEC case(Table 6) for ϵ=-0.05,-0.03,-0.01,0.01,0.03,0.05 are -0.0436,-0.0262,-0.0087,0.0087, 0.0262,0.436 respectively. For the other two cases in BEC, we can gain similar results. While for the matrix perturbation to BEC-like problem, we obtain a much smaller relative errors of eigenvalue for different ϵ. So from the numerical results, we can deduce an approximate formula as follow

$$\frac{\lambda_O - \lambda_p}{\lambda_O} \approx \gamma\epsilon, \quad \text{where} \quad \gamma \in (0,1)$$

which provide us a numerical verification for the perturbation analysis. We conjecture that the size of γ may depend on the sparsity of the matrix **B**.

5.3.2 Random perturbation to matrix B

In reality, the data are in the same noise source, so it is reasonable to assume that the disturbance of data is regular to some extent. In order to reflect reality more, we also consider the random noise to matrix **B**. In this situation, we only describe the case of BEC

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in two dimension. As for the other two cases, we can do the same analysis. For BEC-like NEP, we only test the maximum nonlinear eigenvalue.

Random perturbation to matrix is simulated through the following steps. First, we generate a random matrix $\mathbf{C}$ with the MATLAB code "$randi([a,b],m,n)$", where a, b represent the upper and lower bounds of the values of random matrix elements and m, n denote the dimension of the random matrix. Second, we fix the noise level compared with $\mathbf{B}$ is $\epsilon \in [-0.05, 0.05]$. Third, based on matrix $\mathbf{C}$, we generate the random noise matrix $\mathbf{N}$ with $\mathbf{N} = \epsilon \cdot norm(\mathbf{B})\mathbf{C}$. We declare that, for each n and ϵ, we have done 20 tests. In order to estimate the combined effects of random perturbation, we choose the average of the 20 test results as the final test value.

We remark here that in the two following tables, λ_t denotes the test eigenvalue(mean of 20 tests), while λ_O is the original eigenvalue. Since we use the same data ($\mathcal{A}$, $\mathbf{B}$, $\mathbf{x}_0$) in each n as previously, so we can take λ_O from there directly. For convenience, we show them here. For BEC problem in two dimension case, $n = 10$, $\lambda_O = 22.3486$; $n = 20$, $\lambda_O = 22.4724$; $n = 30$, $\lambda_O = 22.4593$. For BEC-like NEP, $n = 10$, $\lambda_O = 19.1554$; $n = 20$, $\lambda_O = 31.7124$;$n = 30$, $\lambda_O = 42.6003$.

Table 11 matrix $\mathbf{B}$ in BEC problem (2D)is randomly perturbed

ϵ	n=10		n=20		n=30	
	λ_t	$\frac{\|\lambda_t-\lambda_O\|}{\lambda}$	λ_t	$\frac{\|\lambda_t-\lambda_O\|}{\lambda}$	λ_t	$\frac{\|\lambda_t-\lambda_O\|}{\lambda}$
-0.05	22.5044	0.0070	22.4300	0.0019	21.7967	0.0295
-0.03	22.6299	0.0126	22.5635	0.0041	22.0162	0.0203
-0.01	22.2801	0.0031	22.4708	0.0001	22.3252	0.0060
0.01	22.3134	0.0016	22.8175	0.0154	22.0999	0.0160
0.03	21.9848	0.0163	21.6889	0.0349	21.9989	0.0205
0.05	21.4276	0.0412	22.0223	0.0200	22.0451	0.0190

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Table 12 matrix **B** in BEC-like NEP is randomly perturbed

ϵ	n=10		n=20		n=30	
	λ_t	$\frac{\lvert\lambda_t-\lambda_O\rvert}{\lambda}$	λ_t	$\frac{\lvert\lambda_t-\lambda_O\rvert}{\lambda}$	λ_t	$\frac{\lvert\lambda_t-\lambda_O\rvert}{\lambda}$
-0.05	19.1559	0.0213e-3	31.7088	-0.1146e-3	42.5996	0.1937e-4
-0.03	19.1546	0.1945e-3	31.7104	0.0641e-3	42.5999	0.1095e-4
-0.01	19.1544	0.0235e-3	31.7121	0.0084e-3	42.6009	0.0900e-4
0.01	19.1549	0.0539e-3	31.7125	0.0045e-3	42.6007	0.1311e-4
0.03	19.1591	0.0439e-3	31.7138	0.0452e-3	42.5998	0.0900e-4
0.05	19.1558	0.0270e-3	31.7118	0.0202e-3	42.6011	0.1526e-4

From Tables 11 and 12, we can see that the relative error between the original eigenvalue and the test eigenvalue is very small. And it is easy to verify that its value is controlled down below the noise level ϵ, which is consistent with the regular disturbance case. However, we should claim that our inference is valid only in the sense of average. For single random perturbation, the relative error mentioned above may be out of the control of the noise level. We do not know how could this happen. One of explanation is that the random disturbance may change the structure of the matrix a lot, which may lead a influence heavier than the noise level.

Remark 5.3 The regular disturbance in the matrix would make a foreseeable perturbation to the eigenvalue. While the random disturbance would make a more random influence. However, if we take more experiments, we would find out that the average influence of random disturbance is consistent with the regular noise. Actually, it is reasonable to take the mean as test results for the extreme situation is uncommon.

6 Conclusion

We extend SS-HOPM from finding eigenvalue of tensor to solve the nonlinear eigenvalue of BEC-like NEP. SS-HOPM plays a similar role in NEP just as in the tensor case. It can

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guarantee to converge to global optimal eigenvalue in theory for suitable choice of shift α, but not guarantee to converge to the global optimal eigenvalue in practice. From different starting points, we may find different eigenvalues. In order to find out the biggest or smallest eigenvalue, we may need to try multiple starting points to proceed our programm.

We have done some analysis on perturbation of matrix or tensor in BEC problem and BEC-like NEP. The basement is on the symmetrization of the outer product of matrix $\mathbf{B}$ and identity matrix $\mathbf{I}$. Then the nonlinear eigenvalue problem become into a Z-eigenvalue problem of a symmetric tensor. As for the perturbation case of matrix or tensor or both of them, we do the analysis in an uniform frame, and we deduce that the relative error of the eigenvalue is controlled below the noise level.

We present a series of experimental results in the form of tables for BEC problem and more general BEC-like NEP. And the numerical experiments have indicated that the SS-HOPM can find eigenpairs of nonlinear eigenvalue problems in acceptable iterations. Thus, the numerical tests provide us a verification for the convergence of Algorithm SS-HOPM from another angle. However, the SS-HOPM has not perform its best when n is large. Its modification for solving BEC problem in a much bigger scale n is a topic for our future study. Also how to choose a reasonable α in advance is a difficult job, we will propose to choose α adaptively in future work.

We have done some numerical tests to verify the results in perturbation analysis in matrix. In the regular noise case, there is a co-directional relation between eigenvalues and perturbations. In the random noise case, the perturbation would make more elusive influence on the change of eigenvalues in single test. However, in the mean sense, the relative error is under control of noise level as in the regular case too.

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