SOLVING THE GLOBAL OPTIMUM OF A CLASS OF MINIMIZATION PROBLEM∗

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Abstract. We study a special nonconvex optimization problem with a single spherical constraint to find a global minimizer of it. One important application of this problem is the discretized energy functional minimization problem of non-rotating Bose-Einstein condensate (BEC). We solve such a problem by exploiting its characterization as a nonlinear eigenvalue problem with eigenvector nonlinearity (NEPv). We show that with the property of NEPv, any algorithm finding the positive stationary point of this optimization problem actually finds its global minimum. In particular, we can obtain the global convergence to global optimum of alternating direction method of multipliers (ADMM) for this problem. Numerical experiments for applications in BEC validate our theories and demonstrate the effectiveness of ADMM for solving this problem.

Key words. spherical constraint, nonlinear eigenvalue, Bose-Einstein condensation, ADMM

AMS subject classifications. 65K05, 65H17, 65N25

1. Introduction. In this paper, we consider the following nonconvex optimization problem over a single spherical constraint:

\[
\begin{align*}
\min_{x \in \mathbb{R}^n} & \quad \frac{\alpha}{2} \sum_{i=1}^{n} x_i^4 + x^T B x \\
\text{s.t.} & \quad \|x\|_2^2 = 1,
\end{align*}
\]

where \(\alpha > 0\) is a fixed constant and \(B\) is an \(n\) by \(n\) symmetric matrix, with positive diagonal entries and nonpositive off-diagonal entries. An important application of this model is to find the ground state of the non-rotating Bose-Einstein condensation (BEC), which is usually defined as the minimizer of the energy functional minimization problem. After suitable discretization, the matrix \(B\) expresses the sum of the discretized Laplacian operator and a diagonal matrix. See [2] and references therein for details.

BEC has attracted great interest in the atomic, molecule and optical physics community and condense matter community[16, 9]. As one of the major problems in the study of BEC, there are already several popular numerical methods that work well to compute the ground state. One class of these methods has been designed for the nonlinear eigenvalue problem with eigenvector nonlinearity (NEPv), which arises from the Gross-Pitaevskii equation (GPE), such as self-consistent field iteration (SCF)[6], full multigrid method[13], etc. The second class deals with the nonconvex constrained minimization problem, see[22, 4] and references therein. In fact, it is easy to show that NEPv is the first-order optimality condition for this minimization problem. However, to the best of our knowledge, little of them give a theoretical guarantee about whether these methods find the best solution for both NEPv and optimization problem.

Although for algorithms solving nonconvex optimization problems, it is generally difficult to analyze convergence behavior, let alone to guarantee convergence to global

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optimum. Many approaches can be applied to solve certain nonconvex problems with effective numerical results. To deal with the orthogonal constraint, the constraint preserving algorithm was proposed based on the manifold optimization theory, where a curvilinear search approach was introduced combined with Barzilai-Borwein step size\[21, 12\]. In those work, convergence to a stationary point was established under some assumption. However, the manifold techniques are sophisticated and complex for implementation if additional constraints are imposed. Another interest idea is to reformulate the objective function into homogeneous polynomial in tensor form\[11\]. The splitting method using Bregman iteration, which covers the alternating direction method of multipliers (ADMM), was also applied to solve orthogonality constrained problems\[14\] without convergence analysis while presenting numerical results quite well. Zhang et al.\[25\] offered the geometric analysis of (1.1) when $B$ is imposed different structures, such as diagonal and rank-one. They also obtained meaningful results for general matrix $B$ utilizing fourth-order optimality conditions and strict-saddle property. We think for the special case considered in this paper, more specified results can be reached with simpler proof.

Triggered by the nice numerical results with BEC for both NEPv and (1.1), we study the property of the stationary condition for (1.1), to give a hint to the global optimum. It is well known that, without rotation, the ground state can be taken as a real non-negative function, and it corresponds to the smallest eigenvalue of NEPv in physics or partial differential equations theory\[7\]. Taking advandage of the special structure, we give a rather simple proof from the linear algebraic point of view for such kind of results. Similar idea was used in research about optimization of trace ratio by Bai, et al.\[1\]. We first prove that under special structure, the NEPv has unique positive eigenvector corresponding to the smallest eigenvalue, which is exactly a global optimum for (1.1). Then we provide an analysis about global convergence to global minimum of ADMM based on the work of Wang, et al.\[19\].

In this paper, we begin the presentation in section 2 with preliminary. In section 3, we exploit the properties of NEPv corresponding to (1.1) and establish the relationship of positive stationary point and global minimum. In section 4, We start by stating the standard ADMM and then derive global convergence to global optimum for it. Application examples on BEC problem and numerical performance are given in section 5. Concluding remarks are in section 6.

2. Preliminary. In this section, we will define the notations and sort out some basic definitions and facts, which will be used in the subsequent analysis. Throughout the paper, we follow the notation commonly used in numerical linear algebra. A vector $x \geq 0 \ (x \in \mathbb{R}^n)$, stands for $x_i \geq 0 \ (\forall i \in [n])$. $[n]$ denotes $\{1,2,\cdots,n\}$. $\| \cdot \|$ is the norm $\| \cdot \|_2$ for vectors and matrices. For $x \in \mathbb{R}^n$, $|x| = (|x_1|, |x_2|, \cdots, |x_n|)^T$. $B \geq 0$ denotes that $B$ is positive semidefinite. $\lambda_{\min}(B)$ and $\lambda_{\max}(B)$ are the smallest and largest eigenvalue of $B$, respectively.

Let $\mathcal{A}$ be a fourth-order diagonal tensor with all diagonal entries are one, then $\mathcal{A}x^4 = \sum_{i=1}^n x_i^4$, $\mathcal{A}x^3 = (x_1^3, x_2^3, \cdots, x_n^3)^T$ is a vector, and $\mathcal{A}x^2$ is a diagonal matrix with $(x_1^2, x_2^2, \cdots, x_n^2)$ as diagonal entries.

**Definition 2.1 (Irreducibility/Reducibility \[18\]).** A matrix $B \in \mathbb{R}^{n \times n}$ is called reducible, if there exists a nonempty proper index subset $I \subset [n]$, such that

$$b_{ij} = 0, \quad \forall i \in I, \quad \forall j \notin I.$$  

If $B$ is not reducible, then we call $B$ irreducible.
3. Nonlinear eigenvalue problems and global optimum. In this section, we characterize the spherical constraint minimization problem (1.1) by a nonlinear eigenvalue problem with eigenvector nonlinearity, which is in fact the first-order necessary conditions of this constrained problem. First, let us define its Lagrangian function with multiplier $\lambda$:

$$L(x, \lambda) = \frac{\alpha}{2}Ax^4 + x^TBx - \lambda(x^Tx - 1)$$

Then we can get the following nonlinear eigenvector problem (NEPv):

$$(3.1) \begin{cases} \alpha Ax^3 + Bx = \lambda x \\ \|x\|^2_2 = 1 \end{cases}$$

Any $(\lambda, x)$ with $x \neq 0$ satisfying (3.1) is called an eigenpair of the NEPv. $\lambda$ and $x$ are corresponding eigenvalue and eigenvector, respectively. There always exists an eigenpair for (3.1), since (1.1) is to minimize a continuous function over a compact set.

In the following of this section, we give a rather simple proof to specify to which eigenvalue $x$ corresponds. Before that, we need some assumption for the structure of (1.1). Except stated otherwise, the thorough article will be discussed under this assumption.

**Assumption 3.1.** The diagonal entries of $B$ are nonnegative, while the off-diagonal entries are nonpositive. Moreover, $B$ is irreducible.

**Example 3.2.** If the sub-diagonal elements of $B$ are negative, then Assumption 3.1 holds. Furthermore, in this case, the nonnegative eigenvector of (3.1) has no zero entry.

**Proof.** Suppose the nonnegative eigenvector $x \in \mathbb{R}^n$ has some $x_i = 0$, according to (3.1), $b_{ii-1}x_{i-1} + b_{ii+1}x_{i+1}$ has to be zero (let $x_0 = x_{n+1} = 0$). It leads to that $x_{i-1} = 0, x_{i+1} = 0$, and recursively, $x = 0$, which contradicts the definition of eigenvector.

**Example 3.3.** Consider the discretization of the Bose-Einstein condensation (BEC) problem, where the two-dimensional space domain is "L"-like and the boundary value is zero. $\Omega = [0, 1] \times [0, 1] \setminus [0.5, 1] \times [0.5, 1]$. We divide $\Omega$ evenly along both two directions with step $h = \frac{1}{n}$, and choose $n = 6$. Then

$$\tilde{B} = n^2 \cdot \begin{bmatrix} B_1 & \Sigma \\ \Sigma & B_1 \end{bmatrix} = \begin{bmatrix} 4 & -1 & 0 & 0 \\ -1 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} , \quad B_1 = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & -I_5 \\ -I_5 & B_2 \end{bmatrix} , \quad B_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -I_5 \\ 0 & 0 & -1 \end{bmatrix}$$

That is, the columns and rows corresponding to $[0.5, 1] \times [0.5, 1]$ turns to be zero. Then removing these columns and rows, adding a positive diagonal matrix, we obtain $B$. For discretized BEC problem, the Assumption 3.1 is satisfied through the recursively adjacency in the Laplacian operator.
Similar to Chang et al. [8], we define the geometric simplicity for NEPv.

**Definition 3.4 (geometric simple of NEPv).** Let \( \lambda \) be an eigenvalue of NEPv (3.1). We say that \( \lambda \) is geometrically simple if the maximum number of linearly independent eigenvectors corresponding to \( \lambda \) equals one. If we restrict the eigenvector \( x \) on the real space, then we call \( \lambda \) real geometrically simple; if \( x \) is restricted on the complex space, then \( \lambda \) is called complex geometrically simple.

**Lemma 3.5.** Under Assumption 3.1, the eigenpair \((\lambda, x)\) has the following properties:

1. There exists an eigenpair \((\lambda, x)\) with \( x \geq 0 \).
2. The eigenpair \((\lambda, x)\) with \( x \geq 0 \) is unique, and \( x \) contains no zero entries, that is, \( x > 0 \). Denote this \( \lambda \) as \( \lambda_0 \).
3. If \( B \succeq 0 \), then \( \lambda \geq \lambda_0 \geq 0 \), for all eigenvalue \( \lambda \), and \( \lambda_0 \) is real geometrically simple.

**Proof.** We prove this lemma in the case \( \alpha = 1 \), it is obvious that the proof can be generalized for all \( \alpha > 0 \).

1. For any \( x \in \mathbb{R}^n \),
\[
\frac{1}{2}Ax^4 + x^TBx = \frac{1}{2} \sum_i x_i^4 + \sum_{i,j} b_{ij}x_ix_j
\]
(nonpositive off-diagonal of \( B \)) \[ \geq \frac{1}{2} \sum_i |x_i|^4 + \sum_{i,j} b_{ij}|x_i||x_j| \]
\[ = \frac{1}{2}A|x|^4 + |x|^TB|x| \]
Thus, (1.1) has a nonnegative solution.

2. Suppose \( x \) is a nonnegative eigenvector, it actually has no zero element. Otherwise, there exists a set \( I \subset [n], T = [n] \setminus I \) such that \( x_i > 0 \) \( (i \in T) \) and \( x_i = 0 \) \( (i \in I) \). For \( k \in I \), \( b_{kj} = 0 \) \( (j \notin I) \) follows from \( \sum_{j \neq k} b_{kj}x_j = 0 \). It contradicts the assumption that \( B \) is irreducible.

For the uniqueness of eigenpair \((\lambda, x)\) with \( x \geq 0 \), we first prove that the eigenvalue corresponding to nonnegative eigenvector is unique. Suppose \((\lambda, x), (\mu, y) \in \mathbb{R} \times \mathbb{R}_+^n \setminus \{0\} \) are two eigenpairs, then \( x > 0 \), \( y > 0 \), \( \|x\|_2 = \|y\|_2 = 1 \). Denote \( t = \min_i \{ \frac{x_i}{y_i} \} \), then \( 0 < t \leq 1 \) and \( x \geq ty \) with \( x_k = ty_k \) for some \( k \). We have
\[
\lambda x_k = x_k^3 + b_{kk}x_k + \sum_{j \neq k} b_{kj}x_j \leq (ty_k)^3 + b_{kk}(ty_k) + \sum_{j \neq k} b_{kj}(ty_j)
\]
\[ (0 < t \leq 1, \ y_k > 0) \leq ty_k^3 + t(By)_k \]
\[ = t\mu y_k, \]
then \( \lambda \leq \mu \), and as the same we can get \( \mu \leq \lambda \). So \( \lambda = \mu \).

Suppose \((\lambda, x), (\lambda, y) \in \mathbb{R} \times \mathbb{R}_+^n \setminus \{0\} \), we prove that \( x \) and \( y \) must be the same. Similar to the arguments above, we can find a \( t \), satisfying \( 0 < t \leq 1 \), \( x \geq ty \) and \( x_k = ty_k \) for some \( k \). Then
\[
\lambda x_k = x_k^3 + b_{kk}x_k + \sum_{j \neq k} b_{kj}x_j \leq (ty_k)^3 + b_{kk}(ty_k) + \sum_{j \neq k} b_{kj}(ty_j)
\]
\[ \leq ty_k^3 + t(By)_k \]
\[ = t\lambda y_k, \]
Since $\lambda x_k = t\lambda y_k$, $\sum_{j \neq k} b_{kj}(x_j - ty_j) = 0$, with the irreducibility of $B$, we obtain the desired result.

3. Suppose $(\mu, y)$ is an eigenpair, then $\mu > 0$ when $B \succeq 0$. According to $b_{ij} \leq 0 (j \neq i)$, $\mu |y| = |Ay|^3 + By \geq Ay^3 + B |y|$. Since $\mu y_i = y_i^3 + b_{ii}y_i + \sum_{j \neq i} b_{ij}y_j$, if $y_i > 0$,

$$\mu |y_i| = y_i^3 + b_{ii}y_i + \sum_{j \neq i} b_{ij}y_j,$$

if $y_i < 0$, we can prove it as the same. The remaining part for $\mu \geq \lambda_0$ is analogous to the above proof, so we just omit it here.

If $B \succeq 0$ and $(\lambda_0, y)$ satisfies (3.1), then $\lambda_0 = Ay^4 + y^T By$, $\lambda_0 \geq 0$. We also have $\lambda_0 |y| \geq Ay^3 + B |y|$. According to 2., there is an eigenvector $x$ corresponding to $\lambda_0$ which is positive. Again, similar to the proof of 2., there is a $t > 0$ such that $t \leq 1$, $x \geq t|y| \geq 0$ and $x_k = t|y_k|$. 

$$\lambda_0 x_k = x_k^3 + (Bx)_k \leq (t|y_k|)^3 + ((B \cdot t)|y|)_k$$

$$\leq t(|y_k|^3 + (B|y|)_k)$$

$$\leq t\lambda_0 |y_k|,$$

Thus, it holds that $x = |y|, Ay^3 + B |y| = \lambda_0 |y|, \|y\| = 1, |y| > 0$. 

If $y_i > 0$ for some $i$, then

$$(Ay^3 + By)_i = y_i^3 + b_{ii}y_i + \sum_{j \neq i} b_{ij}y_j = |y_i|^3 + b_{ii}|y_i| + \sum_{j \neq i} b_{ij}|y_j|,$$

which leads to the conclusion $y > 0$. For $y_i < 0$, we can get $y < 0$ similarly. Thus, $\lambda_0$ is real geometrically simple.

Remark 3.6. We can prove the existence of the nonnegative optimum from a different aspect [23]. In regard of the semi-definite relaxation of (1.1)

\[
\begin{aligned}
\min \quad & \frac{1}{2} \langle X, AX \rangle + \langle B, X \rangle \\
\text{s.t.} \quad & \text{tr}(X) = 1 \\
& \quad X \succeq 0
\end{aligned}
\]

Lemma 3.7 ([24]). When the off-diagonal entries of $A$ and $B$ are non-positive, (1.1) and (3.2) are equal. If $X$ is an optimum for (3.2), then $x = \sqrt{\text{diag}(X)}$ is an optimum of (1.1).

Proof. If $x$ is a feasible point of (1.1), then $xx^T$ is feasible for (3.2). Let $v(1.1)$ and $v(3.2)$ denote the optimal values of (1.1) and (3.2), respectively, we have $v(3.2) \leq v(1.1)$. On the other hand, if $X$ is a feasible point of (3.2), let $x_i = \sqrt{X_{ii}}$, then $x$ is also a feasible point of (1.1) and

$$\frac{1}{2} Ax^4 + x^T Bx = \frac{1}{2} \sum_{i,j,k,l} a_{ijkl} \sqrt{X_{ii}} \sqrt{X_{jj}} \sqrt{X_{kk}} \sqrt{X_{ll}} + \sum_{i,j} b_{ij} \sqrt{X_{ii}} \sqrt{X_{jj}}$$

$$\leq \frac{1}{2} \sum_{i,j,k,l} a_{ijkl} X_{ij} X_{kl} + \sum_{i,j} b_{ij} X_{ij}$$

$$= \frac{1}{2} \langle X, AX \rangle + \langle B, X \rangle$$

Thus, $v(1.1) \leq v(3.2)$. The claimed results then follows.
Now, we can reach the conclusion that the positive (or negative) eigenvector corresponding to the smallest eigenvalue of NEPv(3.1), is exactly the global optimum of (1.1).

**Theorem 3.8.** The minimal solution \( x \) of (1.1) is a global minimum provided \( x \geq 0 \) (or \( x \leq 0 \)). If \( B \succeq 0 \), the minimization problem (1.1) obtains its global minimum if and only if the minimum is the nonnegative (or nonpositive) eigenvector of (3.1). Furthermore, when restricted with nonnegativity, the nonnegative eigenvector is the only global optimum.

**Proof.** The first part is obvious from Lemma 3.5(1.-2.). If \( B \succeq 0 \), for any global minimum \( x^* \), according to the proof of Lemma 3.5(1.), \( |x^*| \) is also a global minimum. Let \((\lambda, x^*)\) and \((\mu, |x^*|)\) be corresponding eigenpairs, respectively. Then, \( \lambda - \frac{\alpha}{2} A(x^*)^4 = \mu - \frac{\alpha}{2} A(|x^*|)^4 \). We have \( \lambda = \mu \). Combined with Lemma 3.5(3.), we obtain that \( x^* > 0 \) or \( x^* < 0 \).

**Remark 3.9.** Based on Theorem 3.8, we can derive that for any algorithm that can find a stationary point for (1.1), we may check whether the solution is a global optimum by its sign. And if we impose the nonnegativity, those algorithms actually can find the global minimum. For example, in the Newton regularized algorithm for BEC problem proposed by Wu et al.\[22\], we can achieve the nonnegativity by simply taking the absolute value of \( x \) in each outer iteration. With a little modification of the convergence theorem in Wen el al.\[20\], we are still able to guarantee the convergence to a stationary point. Thus, according to our previous arguments, the algorithm can converge to a global optimum.

**Remark 3.10.** We can also prove that \( H = Ax^2 + B - \lambda_0 I \succeq 0 \) as the Lemma 3.5(3.), where \( x \) is the corresponding eigenvector of \( \lambda_0 \). Then according to Theorem 2.1 in Zhang et al.\[25\], we can directly come to the conclusion that \( x \) is a global optimum and all global minimums of (1.1) belong to the equivalence class \([x] = \{y \in \mathbb{R}^n : |y_k| = |x_k|, \forall k \in [n]\}\).

**Remark 3.11.** From the proof of Lemma 3.5, we can see that it is also possible to derive the NEPv characterization in the complex case,

\[
\begin{align*}
\min_{x} & \quad \frac{1}{2} A x^H x + x^H B x, \\
\text{s.t.} & \quad \|x\|_2^2 = 1
\end{align*}
\]

The lemma and theorem discussed above are established utilizing similar techniques. In particular, the smallest eigenvalue has complex geometrically simplicity.

**Remark 3.12.** Before we move to the next section for the algorithm solving the optimization problem, we note that Self-Consistent Field (SCF) is a widely used algorithm to solve NEPv. And according to Cai et al.\[6, Theorem 3.1, Theorem 4.2\], we can derive a rough sufficient condition for NEPv (3.1) to have unique eigenvector \( x^* \) corresponding to smallest eigenvalue and SCF to converge globally to \( x^* \). That is,

\[
0 < \alpha < \frac{\lambda_{\text{max}}(B) - \lambda_{\text{min}}(B)}{3}.
\]

4. **Alternating direction method of multipliers.** The challenge to solve the spherical constraint problem comes from the nonlinear and nonconvex constraint. Penalty methods can be used to avoid handling the spherical constraint directly\[15\], while it usually suffers from slow convergence. Constraint preserving algorithms mentioned above in Remark 3.9 obtain effective performance and convergence analysis about stationary point by Wen and Hu el al.\[21, 12\]. Compared with the orthogonality preserving algorithm, alternating direction method of multipliers (ADMM) can
be coded easily, and for the spherical constraint, its subproblem in algorithm can be solved analytically. We also can give a relatively simple proof for the convergence without involving sophisticated manifold theories.

First, we rewrite (1.1) imposing the nonnegative constraint into the standard ADMM problem as the following:

\[
\begin{cases}
\min_{x \in \mathbb{R}^n} & I_s(x) + f(y) \\
\text{s.t.} & x = y
\end{cases}
\]

where \( S = \{x \| x \|_2 = 1, x \geq 0\} \), \( f(y) = \frac{\alpha}{2} A y^4 + y^T B y \). The augmented lagrangian of (4.1) is:

\[
\mathcal{L}_\rho = I_s(x) + f(y) + w^T (x - y) + \frac{\rho}{2} \| x - y \|_2^2,
\]

for which, the iteration steps are:

\[
\begin{align*}
x^{k+1} &:= \text{Proj}_S(y^k - \frac{w^k}{\rho}) \\
y^{k+1} &:= \text{argmin} (f(y) + w^T (x^{k+1} - y) + \frac{\rho}{2} \| x^{k+1} - y \|_2^2) \\
w^{k+1} &:= w^k + \rho (x^{k+1} - y^{k+1})
\end{align*}
\]

**Lemma 4.1.** \( S = \{x \| x \|_2 = 1, x \geq 0\} \), and the projection onto \( S \) denoted by \( \text{Proj}_S(y) := \text{argmin}_{x \in S} \| x - y \| \), then

\[
\text{Proj}_S(y) = \begin{cases}
\text{Proj}_{R^+}(y)_{\|\text{Proj}_{R^+}(y)\|}, & \text{if max} \left\{ y_i \right\} > 0 \\
\{ \sum_i \alpha_i e_i \mid \sum_i \alpha_i^2 = 1, y_i = 0 \}, & \text{if max} \left\{ y_i \right\} = 0 \\
\{ e_i \mid y_i = \text{max}_j \{ y_j \} \}, & \text{if max} \left\{ y_i \right\} < 0
\end{cases}
\]

where \( e_i = (0, \ldots, 1, \ldots, 0)^T \).

**Proof.** Since \( \| x \|_2 = 1 \), it is obvious that \( \text{argmin}_{x \in S} \| x - y \| \Leftrightarrow \text{argmax}_{x \in S} x^T y \).

Case 1. \( \max_i \{ y_i \} > 0 \). We have for any \( x \geq 0 \), \( \| x \| = 1 \), \( x^T y \leq \sum_{i \in \{y_i > 0\}} x_i y_i \leq \| \text{Proj}_{R^+}(y) \| \), the equality holds when \( x = \frac{\text{Proj}_{R^+}(y)}{\|\text{Proj}_{R^+}(y)\|} \).

Case 2. \( \max_i \{ y_i \} = 0 \). It can be solved similarly as Case 1.

Case 3. \( \max_i \{ y_i \} < 0 \). Begin with

\[
\max_{x_1, x_2} x_1 y_1 + x_2 y_2,
\]

where \( x^2_1 + x^2_2 = 1 \) and \( x_1 \geq 0, x_2 \geq 0 \). It can also be formulated as \( \max_{0 \leq \theta \leq \pi} y_1 \cos \theta + y_2 \sin \theta \). We find that the optimal value is \( \max \{ y_1, y_2 \} \) with \( x = e_1 \) if \( y_1 \geq y_2 \) or otherwise. Assume that it holds with \( x \in \mathbb{R}^n \). For \( x \in \mathbb{R}^{n+1} \), we regard the projection problem as \( \max \max_{0 \leq x_{n+1} \leq 1} x_1 y_1 + \cdots + x_n y_n + x_{n+1} y_{n+1} \), where \( x \in S \).

By induction, the optimal solution will be \( x \in \{ e_i \mid y_i = \text{max}_j \{ y_j \} \} \).

In the rest part of this section, we give the convergence analysis of the standard ADMM for the special spherical constraint optimization problem considered here.
Our analysis is based on the work of Wang et al. [19], which required $f(y)$ in (4.1) to be Lipschitz differentiable with constant $L_f$. The following lemma proves that the sequence $\{y_k\}$ generated by (4.3) is bounded, thus $\nabla f(y)$ only need to have Lipschitz constant in local.

**Lemma 4.2.** For any given initial point $y^0$ and $w^0$, if $\rho$ is sufficiently large, the sequence $\{(x^k, y^k, w^k)\}$ is bounded. In particular, if $\rho > \max\{\|w^0\| - 4\lambda_{\min}(B), 16\alpha + 4(\lambda_{\max}(B) - \lambda_{\min}(B)), -2\lambda_{\min}(B)\}$, $\|y^k\| \leq 2 (\forall k)$.

**Proof.** According to (4.3), we have:

\[
\begin{align*}
\|x^{k+1}\| &= 1 \\
\nabla f(y^{k+1}) - w^k - \rho(x^{k+1} - y^{k+1}) &= 0 \\
\nabla f(y^{k+1}) &= w^k + \rho(x^{k+1} - y^{k+1}) \\
\n\Rightarrow \nabla f(y^{k+1}) &= w^{k+1} \\
\Rightarrow \nabla f(y^{k+1}) + \rho y^{k+1} &= \nabla f(y^k) + \rho x^{k+1} (\forall k \geq 1)
\end{align*}
\]

That is

\[2\alpha A(y^{k+1})^3 + 2By^{k+1} + \rho y^{k+1} = 2\alpha A(y^k)^3 + 2By^k + \rho x^{k+1},\]

combined with $2\alpha A(y^{k+1})^2 + 2B + \rho I$ is positive definite when $\rho > -2\lambda_{\min}(B)$, it leads to

\[
\begin{align*}
y^{k+1} &= (2\alpha A(y^{k+1})^2 + 2B + \rho I)^{-1}(2\alpha A(y^k)^3 + 2By^k) \\
\|y^{k+1}\| &\leq \|2\alpha A(y^k)^3 + 2By^k\| \|(2\alpha A(y^k)^2 + 2B\|\|y^k\| + \rho)\| \\
&\leq \frac{(2\alpha\|y^k\|^2 + 2\lambda_{\max}(B))\|y^k\| + \rho}{2\lambda_{\min}(B) + \rho}.
\end{align*}
\]

For any given initial point $w^0$, we have $\nabla f(y^1) + \rho y^1 = w^0 + \rho x^1$ and $\|y^1\| \leq \frac{\|w^0\| + \rho}{2\lambda_{\min}(B) + \rho}$. Then $\|y^1\| \leq 2$ when $\rho \geq \|w^0\| - 4\lambda_{\min}(B)$. Assume that $\|y^k\| \leq 2$, then there exits constant $\rho > \max\{16\alpha + 4(\lambda_{\max}(B) - \lambda_{\min}(B)), -2\lambda_{\min}(B)\}$, which is independent of the sequence $\{y^k\}$, such that $\|y^{k+1}\| \leq 2$. Thus, the boundedness of $\{(x^k, y^k, w^k)\}$ is obtained.

For completeness, we recall and summary some results of Wang et al. as the following lemma, provided that $\{(x^k, y^k, w^k)\}$ is bounded.

**Lemma 4.3.** [19] For sufficiently large $\rho$, There are constants $C_1(\rho) > 0$ and $C > 0$ such that for all sufficiently large $k$, we have

\[
\begin{align*}
\mathcal{L}_\rho(x^k, y^k, w^k) - \mathcal{L}_\rho(x^{k+1}, y^{k+1}, w^{k+1}) &\geq C_1(\rho)(\|y^{k+1} - y^k\|^2), \\
\|x^{k+1} - y^{k+1}\| &\leq \frac{C}{\rho}\|y^{k+1} - y^k\|.
\end{align*}
\]

**Remark 4.4.** For any given initial point $y^0$, $w^0$, if $\rho$ satisfies the condition in Lemma 4.2 so that $\|y^k\| \leq 2$, we can obtain a local Lipschitz constant $\mathcal{L}_f = 4\alpha + 2\lambda_{\max}(B)$, for $f(y)$. Thus, constant $C$ can be chosen as $L_f$, and if $\rho > 2(L_f + 1)$, (4.5) and (4.6) hold consequently.
Case 1. Prove that converge to some Combined with (4.6) and \( \{x^k, y^k, w^k\} \) generated by the standard ADMM according to (4.3) will converge to \((x^*, y^*, w^*)\), and \( y^* \) is a global optimum of (1.1).

Proof. Since \( \{x^k, y^k, w^k\} \) is bounded, we have \( L_\rho(x^k, y^k, w^k) \) is lower bounded and \( \sum_{k=1}^{\infty} ||y^{k+1} - y^k||^2 < \infty \) resulting from (4.5). This implies that \( \lim_{k \to \infty} ||y^{k+1} - y^k|| = 0 \). If each cluster point \( y^* (y^* \geq 0) \) of \( \{y^k\} \) is an eigenvector of (3.1), then they are the same according to Lemma 3.5. Thus sequence \( \{y^k\} \) converges to some \( y^* \). Combined with (4.6) and \( w^k = \nabla f(y^k) (\forall k \geq 1) \), we also have both \( \{x^k\} \) and \( \{w^k\} \) converge to some \( x^* \) and \( w^* \) with \( y^* = x^* \geq 0 \), \( w^* = \nabla f(y^*) \). Now, we only need to prove that \( y^* \) satisfies the NEPv (3.1). We still denote the convergence subsequence as \( \{x^k, y^k, w^k\} \).

Case 1. \( x^* = y^* > 0 \). There exists \( k_0 \), \( x^k > 0 (\forall k > k_0) \). According to Lemma 4.1, \( x^k = \frac{y^{k-1} - \nabla f(y^{k-1})}{\|y^{k-1} - \nabla f(y^{k-1})\|} \) or \( x^k \in \{ \sum_i \alpha_i c_i \sum_i \alpha_i^2 = 1, \alpha_i \neq 0, (y^{k-1} - \nabla f(y^{k-1}))/\rho \}, \forall i \in [n] \). However the second kind of \( x^k \) is impossible, since for sufficiently large \( k_0 \) and sufficiently large \( \rho \), \( y^{k-1} - \nabla f(y^{k-1})/\rho \neq 0 (\forall k \geq k_0) \). Thus, \( y^* = x^* = \lim_{k \to \infty} x^k = \frac{y^* - \nabla f(y^*)}{\|y^* - \nabla f(y^*)\|} \), that is, \( \nabla f(y^*) = \rho (1 - y^* - \nabla f(y^*))y^* \) and \( \|y^*\| = 1. y^* \) is an eigenvector of (3.1).

Case 2. If there exists a nonempty set \( I \subset [n], T = [n] \setminus I \), such that \( y^* > 0 (i \in T) \) and \( y^* = 0 (i \in I) \). Let \( z = y^* - \nabla f(y^*)/\rho \), then Assumption 3.1 results that there must be a \( z_i > 0 (i \in I) \).

Otherwise, \( \forall i \in I, 0 = z_i = -2 \sum_{j \in j \notin I} b_{ij} y_j^* = -2 \sum_{j \in j \notin I} b_{ij} y_j^* \). This leads to \( \forall j \notin I, b_{ij} = 0 \), which contradicts the irreducibility assumption. Thus \( x^*_i > 0 \) correspondingly, which contradicts \( y^*_i = 0 \). According to the arguments above, we come to the conclusion that \( y^* > 0 \) is an eigenvector of (3.1) and thus a global optimum.

Remark 4.6. According to the proof process of the above three lemmas and theorem, for any given initial point \( y^0, w^0 \), a rough condition of \( \rho \) to be sufficiently large might be \( \rho > \max\{\|u^0\| - 4\lambda_{\min}(B), 16\alpha + 4(\lambda_{\max}(B) - \lambda_{\min}(B)), -2\lambda_{\min}(B), 2(24\alpha + 2\lambda_{\max}(B) + 1), 20\alpha + 5\lambda_{\max}(B)\} \).

Remark 4.7. For brevity, in the next section, we only update \( x \) in the way \( x^{k+1} := \frac{y^k - \nabla f(y^k)}{\|y^k - \nabla f(y^k)\|} \) in numerical experiments, and then check whether entries of the solution have the same sign.

We can obtain that ADMM still has a subsequence converges with this update method, and the limit point is an eigenvector of NEPv similarly as Theorem 4.5. Or according to the Corollary 2 of Wu et al.[19], this limit point \( (x^*, y^*, w^*) \) is a stationary point of the augmented Lagrangian \( L_\rho \). That is,

\[
\begin{align*}
0 &= x^* - y^* \\
0 &= \nabla f(y^*) - w^* \\
0 &= cx^* + w^* \text{ for some } c \in R,
\end{align*}
\]

according to the variational theories[17]. So we can infer that \( y^* \) is also a stationary
point of (1.1).

5. Numerical results. In this section, by application on a special class of BEC problem, we explain our theories about global optimum with numerical experiments and demonstrate the convergence and effectiveness of ADMM for solving this special nonconvex optimization problem.

The energy functional minimization problem of non-rotating BEC is defined as

\[
\begin{aligned}
\min_{\phi} E(\phi(x)) := & \int_{\mathbb{R}^d} \left[ \frac{1}{2} |\nabla \phi(x)|^2 + V(x) |\phi(x)|^2 + \frac{\beta}{2} |\phi(x)|^4 \right] dx, \\
\text{s.t.} & \int_{\mathbb{R}^d} |\phi(x)|^2 dx = 1, \quad E(\phi) < \infty.
\end{aligned}
\]

where \( x \in \mathbb{R}^d \) is the spatial coordinate vector, \( V(x) \) is an external trapping potential, and \( \beta \) is a given constant, see [2]. The minimizer \( \phi^*(x) \) is defined as ground state. We only consider \( \beta > 0 \) in this paper. In most applications of BEC, the harmonic potential is used [4, 5].

\[
V(x) = \begin{cases} 
\gamma_x^2 x^2, & d = 1, \\
\gamma_x^2 x^2 + \gamma_y^2 y^2, & d = 2, \\
\gamma_x^2 x^2 + \gamma_y^2 y^2 + \gamma_z^2 z^2, & d = 3,
\end{cases}
\]

where \( \gamma_x, \gamma_y \) and \( \gamma_z \) are three given positive constants. Using the finite difference, we can reformulate the BEC problem as (1.1). We take \( \beta = 0.5, \gamma_x = \gamma_y = \gamma_z = 1, \) and the space domain \( \Omega = [0, 1], [0, 1]^2, [0, 1]^3, \) for \( d = 1, \) \( d = 2, \) \( d = 3 \) respectively. Then if we choose difference step as \( h = \frac{1}{n} \) and divide the \( \Omega \) evenly along each direction, the coefficient \( \alpha \) in (1.1) will be \( \beta n, \beta n^2, \beta n^3 \) accordingly. And \( B \) is a symmetric positive definite sparse matrix satisfying the Assumption 3.1. With the division getting finer, that is, \( n \) going large, the scale of discretization problem increases rapidly. We refer the reader to [3] for the convergence of this finite difference discretization problem to the original energy functional optimization problem.

We implemented all the following algorithms in MATLAB (Release 2016b) and performed them on a Lenovo laptop with an Intel(R) Core(TM) Processor with access to 8GB of RAM. The solver for the convex subproblem in ADMM was Newton method, and we used Gauss-Seidel method to get the descent direction.

To validate our theorem about the global optimum and the convergence of ADMM for the problem considered here, we first solved the BEC problem with both ADMM and SDP relaxation method. According to Remark 3.6 and Lemma 3.7, the SDP relaxation problem is a convex problem and equivalent to the origin nonconvex problem. So we can regard the value computed from SDP relaxation problem as the global optimization value of (1.1). See Table 5.1. Not surprisingly, the optimal value of ADMM solving the discretized BEC problem is the same as the SDP relaxation method. And the entries of optimizer found by ADMM always have the same sign, which corresponds to the smallest eigenvalue of (3.1). In Figure 5.1, it shows some examples of the discretized ground state computed by ADMM. We also observed from the numerical results, that as \( n \) becomes large, the smallest eigenvalue and optimal value increases. Similar numerical behavior can be seen in Yang, et al. [23]. The theoretical analysis for this phenomena utilizing linear algebraic theory might worth further discussion.

Then, to show the effectiveness of ADMM for solving this spherical constraint optimization problem, we compared it with the Regularized Newton (RN) method proposed by Wu et al. [22] for the two-dimensional case. We refined the mesh from \((2^4+1)\times(2^4+1), (2^5+1)\times(2^5+1) \) to \((2^7+1)\times(2^7+1) \) with the coarse meshes technique
Table 5.1
Numerical results of ADMM on BEC. In the first column, \( d \) represents the space dimension and \( N \) is the number of split points in one direction, including two endpoints. The second column shows the smallest eigenvalue corresponding to the solution computed by ADMM. The third and fourth columns are objective value of ADMM and SDP relaxation method, respectively. The last column check whether the solution obtained by ADMM has all entries with the same sign. Y stands for they indeed have the same sign.

| \( d \) | \( N \) | \( \lambda \) | \( \text{obj} \) | \( \text{sdp obj} \) | \( \text{sign} \) |
|---|---|---|---|---|---|
| 1 | 257 | 5.8214 | 5.4492 | 5.4492 | Y |
| 1 | 513 | 5.8214 | 5.4493 | 5.4493 | Y |
| 2 | 9 | 11.1280 | 10.5802 | 10.5802 | Y |
| 2 | 17 | 11.2246 | 10.6755 | 10.6755 | Y |
| 3 | 5 | 16.0687 | 15.2886 | 15.2868 | Y |
| 3 | 9 | 16.6514 | 15.8564 | 15.8564 | Y |

Fig. 5.1. The discretized ground state computed by ADMM. On the left is for one dimensional space with 513, 1025 total split points, respectively. On the right is the discretized ground state obtained for two dimensional space with 65 split points in each direction.

as [22]. We stopped the ADMM when \( \|x^{k+1} - y^{k+1}\|_2 \leq 10^{-6} \) and \( \|\rho(x^{k+1} - x^k)\|_2 \leq 10^{-6} \). For NR, the stopping criterion is \( \|x^{k+1} - x^k\|_\infty \leq 10^{-6} \). A summary of the results is presented in the Table 5.2. Figure 5.2 illustrates the convergence of value of the objective function via iteration numbers for ADMM and RN more intuitively.

Table 5.2
Comparison between the standard ADMM and RN. The columns of total iter show the number of iterations. For RN method, it includes the iteration of feasible method; for ADMM, it includes the inner iteration for solving the unconstrained convex subproblem, and the numbers in brackets stand for the outer ADMM iteration. The columns of cpu are the cumulative time from the coarsest mesh. The nrmG column is \( \|\nabla f(x) - (x^T \nabla f(x))x\| \), where \( x \) is the computed optimizer, \( f(x) \) is the objective function.

| \( N \) | \( \text{total iter} \) | \( \text{cpu(s)} \) | \( \text{obj val} \) | \( \text{nrmG} \) | \( \text{total iter} \) | \( \text{cpu(s)} \) | \( \text{obj val} \) | \( \text{nrmG} \) |
|---|---|---|---|---|---|---|---|---|---|
| 17 | 64 | 0.1042 | 10.6755 | 1.28e-4 | 54(26) | 0.0414 | 10.6755 | 7.39e-4 |
| 33 | 58 | 0.2707 | 10.6994 | 1.45e-4 | 30(16) | 0.1007 | 10.6994 | 3.78e-4 |
| 65 | 66 | 3.5692 | 10.7054 | 2.36e-4 | 30(16) | 0.4462 | 10.7054 | 1.99e-4 |
| 129 | 62 | 61.4100 | 10.7069 | 4.98e-4 | 42(16) | 4.3061 | 10.7069 | 9.98e-4 |

From the numerical results of the comparison, ADMM needs rather fewer total iterations to converge and thus fewer time to obtain a satisfying solution. We also
found that although ADMM takes fewer total iterations, the inner iteration is not as efficient as expected for large scale problems. An obvious deficiency is to solve a linear system in each inner iteration for Newton method. For the discretized BEC problem, we may take the advantage of the structure of Laplacian operator to solve the linear system more efficiently. This will be our future work.

6. Concluding Remarks. We considered a special nonconvex optimization problem over a spherical constraint and characterized it with a nonlinear eigenvalue problem with eigenvector nonlinearity (NEPv). The properties of NEPv were studied. Attention was paid to the smallest eigenvalue, which corresponds to a unique nonnegative (nonpositive) eigenvector. We established the equivalence between this eigenvector and the global optimum, which can help to determine whether a stationary point found by algorithms is a global optimum. The standard ADMM for this nonconvex minimization problem has proven global convergence to the global minimum. We validated our theories and demonstrated the effectiveness of the standard ADMM by numerical experiments arising in the discretized non-rotating BEC problem.

The results presented in this work depend on the structure of $B$ strongly. The nonpositivity off-diagonal and irreducibility allow us to employ the eigenvector characterization in Theorem 3.8. And various algorithms, particularly the ADMM turned out to be convergent to global optimum when they are utilized to solve BEC problems. However, it might be too strict. For instance, the BEC problem with sine pseudospectral discretization can also be solved similarly resulting good numerical results, while our assumption not covers it. How to solve the problem when this assumption is relaxed is a subject of future study. Also as already mentioned, another future work will be the improvement of algorithms for solving the BEC-like problem in large scale, including general accelerated schemes of ADMM, such as [10], dealing with the large scale linear system for the subproblem utilizing the structure of discretized Laplacian operator and generalizing the convergence analysis for them.

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