• **ARTICLES** • doi:

A Note on Semidefinite Programming Relaxations For Polynomial Optimization Over a Single Sphere

Jiang Hu[1,*], Bo jiang[2], Xin Liu[3] & Zaiwen Wen[1]

[1] *Beijing International Center for Mathematical Research, Peking University, Beijing* 100871*, CHINA;*
[2] *Research Center for Management Science and Data Analytics, School of Information Management and Engineering, Shanghai University of Finance and Economics, Shanghai* 200433 *CHINA;*
[3] *Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing* 100190 *CHINA;*
Email:jianghu@pku.edu.cn, jiang.bo@mail.shufe.edu.cn, liuxin@lsec.cc.ac.cn, wenzw@pku.edu.cn

Received ; accepted

Abstract In this paper, we study two instances of polynomial optimization problem over a single sphere. One problem is to compute the best rank-1 tensor approximation. We show the equivalence between two recent semidefinite relaxations methods. The other problem arises from Bose-Einstein condensates, whose objective function is a summation of a probably nonconvex quadratic function and a quartic term. We show that this problem is NP-complete and propose a semidefinite relaxation with both deterministic and randomized rounding procedures. Explicit approximation ratios for these rounding procedures are presented. Preliminary numerical experiments are performed to show the quality of these semidefinite relaxations.

Keywords Polynomial Optimization Over a Single Sphere, Semidefinite Programming, Best Rank-1 Tensor Approximation, Bose-Einstein condensates

MSC(2010) 65K05, 90C22, 90C26

Citation: Jiang H, Bo J, Xin L, Zaiwen W. SCIENCE CHINA Mathematics journal sample. Sci China Math, 2013, 56, doi: 10.1007/s11425-000-0000-0

1 Introduction

In this paper, we consider two specific instances of minimizing a polynomial function over a single sphere as

$$\min_{x\in\mathbb{R}^n} \quad f(x) \quad \text{s. t.} \quad \|x\|=1, \tag{1.1}$$

where f is a real-valued polynomial function and the norm is the Euclidean norm. The variable x may be in the complex domain. This problem is widely used in tensor rank approximations and decompositions, Bose-Einstein condensates (BECs) and many other problems. Moreover, it also plays an important role in signal processing, speech mechanics, biomedical engineering and quantum mechanics [9, 20, 23].

There are many generic methods for solving (1.1). Since it is a differentiable nonlinear programming problem [21], the classic methods, such as the quadratic penalty method, the augmented Lagrangian method and the sequential quadratic programming methods, can be applied to find stationary points or even local minimizers of (1.1). On the other hand, noting that the collection of all vectors with unit norms is a special form of the Stiefel manifold, problem (1.1) can be solved by the methods for optimization on manifolds [1]. In particular, a feasible method is proposed in [14] for optimization with orthogonality

*Corresponding author

constraints and it has been applied successfully in applications such as genus-0 surface mapping and density functional theory.

When f is a homogeneous polynomial, problem (1.1) is closely related to the rank-1 tensor approximations and there are quite a few specialized methods. A higher-order power method (HOPM) is proposed in [9]. Although it works well in many cases but may not converge in symmetric generalization. A symmetric HOPM is presented in [16] and its convergence can be guaranteed under certain conditions. It is reported in [22] that the convergence to a stationary point of a shifted symmetric HOPM can be ensured. In [20], the tensor relaxation methods and polynomial-time approximation algorithms with high approximation ratios are developed. The approximation ratios are further improved in [18,19]. The Z-eigenvalues of tensors are studied in [17] and a method is designed by solving a sequence of semidefinite relaxations based on sum of squares (SOS) representations. The local methods mentioned above are easy to be implemented. Recently, Nie and Wang [7] propose a semidefinite programming (SDP) relaxation approach based on SOS. Jiang, Ma and Zhang [8] provide another SDP relaxation by using the matricization of the tensor. These two methods can identify the global solutions under certain conditions.

The BEC problem has been extensively studied in the atomic, molecule and optical (AMO) physics community and condense matter community. Under a suitable discretization of the energy functional and constraints, it can be formulated as (1.1). Specifically, the objection function $f(x)$ is a summation of a quadratic function and a simple quartic term. Although the BEC problem looks concise, solving it efficiently is a numerical challenge since the total number of variables can easily be more than one million and the Hessian matrix can be indefinite in the complex domain, in particular, when two parameters in the energy functional are large. Various gradient projection methods have been developed for solving the BEC problem. A normalized gradient flow method via the backward Euler finite difference or Fourier (or sine) pseudospectral discretization method has been extended to compute ground states of spin-1 BEC [2,3], dipolar BEC [5] and spin-orbit coupled BEC [4]. A new Sobolev gradient method is developed in [6]. Recently, a regularized Newton method is proposed in [15] by replacing the objective function by its second-order Taylor expansion and adding a proximal term.

This paper is divided into two parts. The first part is to study the two SDP relaxations proposed accordingly in [7] and [8] for the best rank-1 tensor approximation. Although their formulations look quite different, by reviewing and comparing them carefully, we find that they are indeed equivalent in the sense that the same object is represented in two different ways. Specifically, the size of matrix variable in SDP from [7] is smaller than that of [8] since many redundant variables are removed in [7] by exploiting certain symmetric property. It is worth mentioning that in the presence of some other constraints, usually both aforementioned SDP relaxations may not work. Meanwhile, the nuclear norm penalty approach in [8] can still provide a low-rank even rank-1 solution.

The second part of the paper focuses on the BEC problem. We prove that the BEC problem is NP-Complete by establishing its connection to the partition problem. Since it can be formulated as a specific instance of the best rank-1 tensor approximations, the above two generic SDP relaxation approaches can be applied to the BEC problems directly. However, the size of the problem grows exponentially with the increase of the dimension of the original variable. Consequently, solving these SDP relaxations becomes practically intractable. Therefore, we propose a quadratic SDP relaxation with significantly smaller size. Then approximate solutions to the BEC problem can be constructed by both deterministic and randomized rounding procedures from the SDP solutions. The deterministic approach ensures an approximation ratio less than r, where r is the rank of the SDP solution. The randomized approach draw a random vector from the i.i.d Gaussian distribution. Although the numerical advantage of this randomized version has not been observed, the probability of obtaining a solution with an assured quality is dimensional free. Finally, preliminary numerical experiments are reported to verify our observation.

Notations. The symbol $\mathbb{N}$ denotes the set of nonnegative integers. Given the tensors $\mathcal{X}, \mathcal{Y} \in \mathbb{R}^{n_1 \times n_2 \times \cdots \times n_m}$ and $\mathcal{Z} \in \mathbb{R}^{n_{m+1} \times n_{m+2} \times \cdots \times n_{m+l}}$, we define the inner product

$$\langle \mathcal{X}, \mathcal{Y} \rangle = \sum_{1 \leqslant i_1 \leqslant n_1, \cdots, 1 \leqslant i_m \leqslant n_m} \mathcal{X}_{i_1, \cdots, i_m} \mathcal{Y}_{i_1, \cdots, i_m}$$

and the outer product

$$(\mathcal{X} \otimes \mathcal{Z})_{i_1,\cdots,i_{m+l}} = \mathcal{X}_{i_1,\cdots,i_m}\mathcal{Z}_{i_{m+1},\cdots,i_{m+l}},$$

which is a tensor of order $m + l$. The trace of a matrix A is denoted by $\mathrm{tr}(A)$. For a vector of indices $\alpha = (\alpha_1, \cdots, \alpha_n) \in \mathbb{N}^n$, we define $|\alpha| = \alpha_1 + \cdots + \alpha_n$ and $\mathbb{N}^n_m = \{\alpha \in \mathbb{N}^n : |\alpha| = m\}$. Let $\pi(i_1, \cdots, i_m)$ be a permutation of the tuples $(i_1, \cdots, i_m)$. A tensor $\mathcal{F} \in \mathbb{R}^{n_1\times\cdots\times n_m}$ is symmetric if $n_1 = \cdots = n_m$ and $\mathcal{F}_{\pi(i_1,\cdots,i_m)} = \mathcal{F}_{i_1,\cdots,i_m}$. We define the norm of $\mathcal{F}$ by $||\mathcal{F}|| = (\sum\limits_{i_1=1}^{n_1} \cdots \sum\limits_{i_m=1}^{n_m} |\mathcal{F}_{i_1,\cdots,i_m}|^2)^{1/2}$. For a tensor $\mathcal{F}$ of order m, there exists tuples $(u^{i,1}, \cdots, u^{i,m})$ $(i = 1, \cdots, r)$, where $u^{i,j} \in \mathbb{C}^{n_j}$, such that $\mathcal{F}$ can be expressed as

$$\mathcal{F} = \sum_{i=1}^{r} u^{i,1} \otimes \cdots \otimes u^{i,m}.$$

The smallest r in the above equation is called the rank of $\mathcal{F}$.

The rest of this paper is organized as follows. We introduce the best rank-1 tensor approximation, review the two SDP relaxations and establish their equivalence in Section 2. The SDP relaxation based approaches for the BEC problem are studied in section 3. Numerical results on the equivalence of the two SDP relaxations and comparisons between different SDP relaxations for solving the BEC problem are presented in Section 4.

2 The Equivalence Between Two SDP Relaxation Methods

Recently, there are two approaches based on semidefinite programming relaxation for finding the global optimal solution of the best rank-1 tensor approximation problem. A lot of numerical results suggest that both of these two relaxations are very likely to be tight. In fact, this is not a coincidence. In this section, we review them and establish their equivalence.

2.1 Best Rank-1 Tensor Approximation

An mth-order tensor $\mathcal{F} \in \mathbb{R}^{n_1\times n_2\times\cdots\times n_m}$ is a multi-dimensional array whose indices $(i_1, i_2, \cdots, i_m)$ are $1 \leqslant i_1 \leqslant n_1, \cdots, 1 \leqslant i_m \leqslant n_m$. Obviously, the 1st-order and 2nd-order tensors are regular vectors and matrices, respectively. If an mth-order tensor $\mathcal{X}$ is rank one, the definition of the rank of tensors yields an expression $\mathcal{X} = \lambda \cdot x^1 \otimes x^2 \otimes \cdots \otimes x^m$ for some $\lambda \in \mathbb{R}$ and $x^1 \in \mathbb{R}^{n_1}, \cdots, x^m \in \mathbb{R}^{n_m}$. For a given tensor $\mathcal{F} \in \mathbb{R}^{n_1\times n_2\times\cdots\times n_m}$, finding the best rank-1 tensor approximations of $\mathcal{F}$ can be expressed as

$$\min_{\mathcal{X}\in\mathbb{R}^{n_1\times n_2\times\cdots\times n_m}} \|\mathcal{F} - \mathcal{X}\|^2 \quad \text{s. t.} \quad \mathrm{rank}(\mathcal{X}) = 1, \tag{2.1}$$

which is equivalent to

$$\min_{\lambda,x^1,\ldots,x^m} \quad \|\mathcal{F} - \lambda \cdot x^1 \otimes \cdots \otimes x^m\|^2 \quad \text{s. t.} \quad \lambda \in \mathbb{R}, \quad ||x^1|| = \cdots = ||x^m|| = 1. \tag{2.2}$$

The Lagrangian function of (2.2) is

$$L = \sum_{i_1 i_2\cdots i_m} (\mathcal{F}_{i_1 i_2\cdots i_m} - \lambda x^1_{i_1} x^2_{i_2} \cdots x^m_{i_m})^2 + \sum_{j=1}^{m} \pi^j \left(\sum_{i_j=1}^{n_j} (x^j_{i_j})^2 - 1 \right),$$

where $\pi^i (1 \leqslant i \leqslant m)$ are the Lagrangian multipliers corresponding to the constraints $\|x^i\| = 1$, respectively. Taking derivatives of L with respect to the variables x^i and λ and setting them to zero leads to the first-order optimality conditions. A simple linear algebraic calculation from these conditions gives

$$\sum_{i_1 i_2\cdots i_m} \mathcal{F}_{i_1 i_2\cdots i_m} x^1_{i_1} x^2_{i_2} \cdots x^m_{i_m} = \lambda. \tag{2.3}$$

Then the objective function of (2.2) becomes

$$\|\mathcal{F} - \lambda \cdot x^1 \otimes \cdots \otimes x^m\|^2 = ||\mathcal{F}||^2 + \lambda^2 - 2\lambda \cdot \sum_{i_1 i_2 \cdots i_m} \mathcal{F}_{i_1 i_2 \cdots i_m} x^1_{i_1} x^2_{i_2} \cdots x^m_{i_m} = ||F||^2 - \lambda^2.$$

Since $||\mathcal{F}||$ is a constant for a given $\mathcal{F}$, the problem (2.3) is equivalent to

$$\begin{cases} \max\limits_{x^1 \in \mathbb{R}^{n_1}, \cdots, x^m \in \mathbb{R}^{n_m}} |F(x^1, \cdots, x^m)| \\ \quad \text{s. t.} \quad \|x^1\| = \cdots = \|x^m\| = 1, \end{cases} \tag{2.4}$$

where $F(x^1, \cdots, x^m) = \sum\limits_{i_1 i_2 \cdots i_m} \mathcal{F}_{i_1 i_2 \cdots i_m} x^{(1)}_{i_1} x^{(2)}_{i_2} \cdots x^{(m)}_{i_m}$. Hence, a rank-1 tensor $\lambda \cdot (u^1 \otimes \cdots \otimes u^m)$ with $\lambda \in \mathbb{R}$ and $\|u^i\| = 1$ $(i = 1, \ldots, m)$ is a best rank-1 approximation of the tensor $\mathcal{F}$ if and only if $(u^1, \cdots, u^m)$ is a global maximizer of (2.1) and $\lambda = F(u^1, \cdots, u^m)$.

When $\mathcal{F}$ is symmetric, it is shown in [10] that (2.1) always has an optimal symmetric tensor solution. In fact, (2.4) reduces to

$$\max_{x \in \mathbb{R}^n} \quad |f(x)| \quad \text{s. t.} \quad x^\top x = 1, \tag{2.5}$$

where $x = x^1 = \cdots = x^m$, and $f(x) = F(x, \cdots, x)$. It can verified that $\lambda \cdot x \otimes \cdots \otimes x$ is the best symmetric tensor if and only if x is a global maximizer of (2.5) and $\lambda = f(x)$. Therefore, the best rank-1 tensor approximation is converted to a polynomial function optimization problem over a single sphere as (1.1).

Suppose that $\mathcal{F}$ is an mth-order nonsymmetric tensor. One can construct a symmetric tensor $\mathcal{T}$ as

$$\mathcal{G}_{i_1 \cdots i_m} = \begin{cases} \mathcal{F}_{j_1 \cdots j_m}, & \text{if } 1 + \sum\limits_{l=1}^{k-1} n_l \leqslant i_k \leqslant \sum\limits_{l=1}^{k} n_l \text{ and } j_k = i_k - \sum\limits_{l=1}^{k-1} n_l \\ 0, & \text{otherwise,} \end{cases},$$

$$\mathcal{T}_{i_1 \cdots i_m} := \frac{1}{|\pi(i_1, \cdots, i_m)|} \sum_{j_1 \cdots j_m \in \pi(i_1 \cdots i_m)} \mathcal{G}_{j_1 \cdots j_m}, \quad \forall 1 \leqslant i_1, \cdots, i_m \leqslant \sum_{l=1}^{m} n_l,$$

where $\mathcal{G}$ and $\mathcal{T}$ are m-order tensor of dimension $n_1 + \cdots + n_m$. Here, $\mathcal{T}$ is the symmetric form $\mathcal{G}$. Hence, we can obtain the best rank-1 approximation of $\mathcal{T}$ by using the symmetric tensor methods. Once we find the best rank-1 tensor $\lambda \cdot \underbrace{y \otimes \cdots \otimes y}_{m}$ of $\mathcal{T}$, then $\lambda \cdot x^1 \otimes \cdots \otimes x^m$ is the best rank-1 approximation of $\mathcal{F}$, in which $x^1, \cdots, x^m$ satisfying $y = ((x^1)^\top, \cdots, (x^m)^\top)^\top$, with dimension $n_1, \cdots, n_m$. Therefore, problems on finding the best rank-1 tensor approximations of $\mathcal{F}$ and $\mathcal{T}$ are equivalent to some extent.

Suppose that $\mathcal{F}$ is an $(2d+1)$-order symmetric tensor. A $4d$-th symmetric tensor $\mathcal{G}$ can be constructed as

$$\mathcal{G}_{i_1, \cdots, i_{4d}} = \frac{1}{|\pi(i_1, \cdots, i_{4d})|} \sum_{k=1}^{n} \left(\sum_{j_1 \cdots j_{4d} \in \pi(i_1 \cdots i_{4d})} \mathcal{F}_{i_1 \cdots i_{2d} k} \mathcal{F}_{i_{2d+1} \cdots i_{4d} k} \right).$$

Then (2.4) is equivalent to

$$\begin{cases} \max\limits_{x} & \mathcal{G}(x, \cdots, x) \\ \text{s. t.} & \|x\| = 1. \end{cases}$$

Another approach is to add a new variable x_{n+1} and define $\tilde{x} := (x_1, \cdots, x_n, x_{n+1})$ and $\tilde{f}(\tilde{x}) := f(x) x_{n+1}$. Then $\tilde{f}(\tilde{x})$ is a form of even degree $2d+2$, which yields the optimization problem:

$$\tilde{f}_{\max} := \max_{\tilde{x} \in \mathbb{R}^{n+1}} \tilde{f}(\tilde{x}) \quad \text{s. t.} \quad \|\tilde{x}\| = 1. \tag{2.6}$$

Using the relationship

$$f_{\max} = \sqrt{2d+1} (1 - \frac{1}{2(d+1)})^{-d-1} \tilde{f}_{\max},$$

we can easily obtain the optimal solutions from (2.6).

Combining all facts above, we conclude the best rank-1 tensor approximations for both symmetric and nonsymmetric tensors can be identified as long as the symmetric case is solvable.

2.2 Nie-Wang's SDP Relaxation Approach [7]

For an mth-order symmetric tensor $\mathcal{F}$, Nie and Wang solve (2.5) by maximizing and minimizing $f(x)$ over the spherical constraint, respectively. Specifically, the maximizing problem is

$$f_{\max} := \max_{x\in\mathbb{R}^n} \quad f(x) \quad \text{s. t.} \quad x^\top x = 1. \tag{2.7}$$

Let $m = 2d$, $c := \{c_\alpha\}$ and $g := \{g_\alpha\}$ be the coefficients of the polynomial functions $f(x)$ and $(x^\top x)^d$ such that

$$f(x) := \sum_{\alpha\in\mathbb{N}^n_m} c_\alpha x^\alpha, \quad (x^\top x)^d := \sum_{\alpha\in\mathbb{N}^n_m} g_\alpha x^\alpha.$$

Introducing a vector $[x^d] := [x_1^d, \ \ x_1^{d-1}x_2, \cdots, x_1^{d-1}x_n, \cdots, x_n^d]^\top$ of length $\binom{n+d-1}{d}$, we obtain a square matrix

$$M \quad := \quad [x^d][x^d]^\top = \sum_{\alpha\in\mathbb{N}^n_m} A_\alpha x^\alpha, \tag{2.8}$$

where A_α is a symmetric matrix with dimensions $\binom{n+d-1}{d} \times \binom{n+d-1}{d}$.

For each moment function x^α where $\alpha \in \mathbb{N}^n_m$, we can assign a linear variable y_α to replace x^α. Given $y \in \mathbb{R}^{\mathbb{N}^n_m}$, we define linear functions

$$\langle c, y\rangle = \sum_{\alpha\in\mathbb{N}^n_m} c_\alpha y_\alpha, \quad \langle g, y\rangle := \sum_{\alpha\in\mathbb{N}^n_m} g_\alpha y_\alpha, \quad M_1(y) := \sum_{\alpha\in\mathbb{N}^n_m} A_\alpha y_\alpha.$$

Therefore, problem (2.7) is equivalent to

$$\max_{y\in\mathbb{R}^{\mathbb{N}^n_m}} \langle c, y\rangle \quad \text{s. t.} \quad M_1(y) \succeq 0, \quad \langle g, y\rangle = 1, \quad \operatorname{rank}(M_1(y)) = 1.$$

Removing the rank-1 constraint yields a semidefinite programming relaxation to (2.7) as follows

$$f^{\text{sdp}}_{\max} := \max_{y\in\mathbb{R}^{\mathbb{N}^n_m}} \langle c, y\rangle \quad \text{s. t.} \quad M_1(y) \succeq 0, \quad \langle g, y\rangle = 1. \tag{2.9}$$

Since $\operatorname{tr}(M_1(y)) \leqslant \langle g, y\rangle = 1$, the optimal solution of (2.9) always exists. Suppose that y^* is a maximizer. An approximate solution can be constructed from y^* as follows. We first find an index s such that $y^*_{2de_s} = \max\limits_{1\leqslant i\leqslant n} y^*_{2de_i}$, where e_i is the vector whose ith entry equals to one and all other entries are equal to zero. Then, we compute

$$x = \hat{u}/\|\hat{u}\|, \lambda = f(x). \tag{2.10}$$

where $\hat{u} = (y_{(2d-1)e_s+e_1}, \cdots, y_{(2d-1)e_s+e_n})$. The vector x is an exact maximizer if $M(y^*) = 1$ and it is usually a good approximation when $M(y^*) \geqslant 1$. The case on minimizing $f(x)$ over the spherical constraint can be obtained in the same fashion.

2.3 Jiang-Ma-Zhang's SDP Relaxation Approach [8]

Jiang, Ma and Zhang [8] reformulated (2.5) by embedding the tensor to a square matrix. Let $\mathcal{X} = x \otimes \cdots \otimes x$. Then we have $f(x) = \langle \mathcal{F}, x \otimes \cdots \otimes x\rangle = \langle \mathcal{F}, \mathcal{X}\rangle$ and

$$\|x\|^{2d} = (x_1^2 + \cdots + x_n^2)^d = \sum_{k\in\mathbb{N}^n_d} \frac{d!}{\prod_{j=1}^n k_j!} \mathcal{X}_{1^{2k_1}2^{2k_2}\cdots n^{2k_n}} = 1.$$

Therefore, problem (2.5) is expressed as

$$\begin{cases} \max & \langle \mathcal{F}, \mathcal{X}\rangle \\ \text{s. t.} & \displaystyle\sum_{k\in\mathbb{N}^n_d} \frac{d!}{\prod_{j=1}^n k_j!} \mathcal{X}_{1^{2k_1}2^{2k_2}\cdots n^{2k_n}} = 1, \\ & \mathcal{X} \in S^{n^{2d}}, \operatorname{rank}\mathcal{X} = 1, \end{cases} \tag{2.11}$$

where S^{n^m} is the set of $\underbrace{n \times n \times \cdots \times n}_{m}$ symmetric tensors. A square matricization operation $M_2(\mathcal{F}) \in \mathbb{R}^{n^d \times n^d}$ of a symmetric $2d$-order tensor $\mathcal{F} \in S^{n^{2d}}$ is further introduced by

$$M_2(\mathcal{F})_{kl} := \mathcal{F}_{i_1 \cdots i_d i_{d+1} \cdots i_{2d}}, 1 \leqslant i_1, \cdots i_d, i_{d+1}, \cdots i_{2d} \leqslant n, \tag{2.12}$$

where

$$k = \sum_{j=1}^{d} (i_j - 1) n^{d-j} + 1, \text{and } l = \sum_{j=d+1}^{2d} (i_j - 1) n^{2d-j} + 1.$$

It follows from the definition that

$$\operatorname{tr}(M_2(\mathcal{X})) = \sum_{k \in \mathbb{N}_d^n} \frac{d!}{\prod_{j=1}^n k_j!} \mathcal{X}_{1^{2k_1} 2^{2k_2} \cdots n^{2k_n}}, \text{ and } \langle M_2(\mathcal{F}), M_2(\mathcal{X}) \rangle = \langle \mathcal{F}, \mathcal{X} \rangle.$$

Since $\operatorname{rank}(\mathcal{X}) = 1$ is equivalent to $\operatorname{rank}(M_2(\mathcal{X})) = 1$, problem (2.11) can be converted into the following equivalent matrix optimization problem:

$$\begin{cases} \max & \langle F, X \rangle \\ \text{s. t.} & \operatorname{tr}(X) = 1, \quad M_2^{-1}(X) \in S^{n^{2d}}, \\ & X \in S^{n^d \times n^d}, \quad \operatorname{rank}(X) = 1, \end{cases} \tag{2.13}$$

where $X = M_2(\mathcal{X}), F = M_2(\mathcal{F})$, and $S^{n^d \times n^d}$ denotes the set of $n^d \times n^d$ symmetric matrices. Removing the rank-1 constraint yields the following SDP relaxation:

$$\begin{cases} \max & \langle F, X \rangle \\ \text{s. t.} & \operatorname{tr}(X) = 1, \\ & M_2^{-1}(X) \in S^{n^{2d}}, \quad X \succeq 0. \end{cases} \tag{2.14}$$

2.4 Equivalence

In this subsection, we establish the equivalence between (2.9) and (2.14). The main concept is to clarify the relationship between the two matrices $M_1(y)$ and $M_2(\mathcal{X})$. Briefly speaking, the matricization (2.12) leads to

$$X = M_2(\mathcal{X}) = [\hat{x}^d][\hat{x}^d]^T = \sum_{\alpha \in \mathbb{N}_m^n} B_\alpha x^\alpha, \tag{2.15}$$

where $[\hat{x}^d]$ is a vector of length n^d whose elements are all possible combinations of the form

$$\{x_{i_1} x_{i_2} \cdots x_{i_d} \mid 1 \leqslant i_j \leqslant n, j = 1, \ldots, d\}$$

and B_α is a symmetric matrix with dimensions $n^d \times n^d$. The main difference is that $[x^d]$ in (2.8) is a sub-vector of $[\hat{x}^d]$ in (2.15) by removing the duplicated elements. Hence, there are more redundancy in $M_2(\mathcal{X})$ than that in $M_1(y)$.

In fact, the entries of M in (2.8) can be expressed as

$$M_{k,l} = x_{i_1} \cdots x_{i_d} x_{i_{d+1}} \cdots x_{i_{2d}}, \ 1 \leqslant i_1 \leqslant \cdots \leqslant i_d \leqslant n, 1 \leqslant i_{d+1} \leqslant \cdots \leqslant i_{2d} \leqslant n,$$

$$\begin{aligned} k &= \sum_{j=1}^{d} \sum_{k_{d-j} = n - i_j + 2}^{n - i_{j-1} + 1} \sum_{k_{d-j-1} = 1}^{k_{d-j}} \cdots \sum_{k_0 = 1}^{k_1} 1 + 1 \ (i_0 := 1), \\ l &= \sum_{j=d+1}^{2d} \sum_{k_{2d-j} = n - i_j + 2}^{n - i_{j-1} + 1} \sum_{k_{2d-j-1} = 1}^{k_{d-j}} \cdots \sum_{k_0 = 1}^{k_1} 1 + 1 \ (i_d := 1). \end{aligned} \tag{2.16}$$

It can be verified that the entries of the matrix X in (2.15) are:

$$X_{k,l} = \; x_{i_1} \cdots x_{i_d} x_{i_{d+1}} \cdots x_{i_{2d}}, \; 1 \leqslant i_1, \cdots, i_d, i_{d+1}, \cdots, i_{2d} \leqslant n.$$

where

$$k = \sum_{j=1}^{d} (i_j - 1) n^{d-j} + 1, \text{ and } l = \sum_{j=d+1}^{2d} (i_j - 1) n^{2d-j} + 1. \tag{2.17}$$

Both of the two SDP relaxations can obtain an optimal solution of the original problem when its SDP solution is rank-1.

We next prove the equivalence between the two SDP problems. For convenience, we define two sets

$$\begin{aligned} \Phi &:= \left\{ Y \in S^{\binom{n+d-1}{d} \times \binom{n+d-1}{d}} \mid Y = \sum_{\alpha \in \mathbb{N}^n_m} y_\alpha A_\alpha, \; y \in \mathbb{R}^{\binom{n+2d-1}{2d}} \right\}, \\ \Psi &:= \left\{ Y \in S^{n^d \times n^d} \mid Y = \sum_{\alpha \in \mathbb{N}^n_m} y_\alpha B_\alpha, \; y \in \mathbb{R}^{\binom{n+2d-1}{2d}} \right\}. \end{aligned}$$

Following the relationships between the matrices A_α and B_α, we establish mappings between the matrices in the sets Φ and Ψ. Let n, d be two integers. A map $\tau: \; \Phi \to \Psi$ is defined as follows. For every matrix $X = \sum_{\alpha \in \mathbb{N}^n_m} y_\alpha A_\alpha \in \Psi$, we define $\bar{X} = \tau(X) = \sum_{\alpha \in \mathbb{N}^n_m} y_\alpha B_\alpha$. Based on the map τ, we can further clarify the relationship between the optimization variables in (2.9) and (2.14). Let $y \in \mathbb{R}^{\mathbb{N}^n_m}$ and $Y \in \Psi$. For $y \in \mathbb{R}^{\mathbb{N}^n_m}$, we introduce a map $\sigma: \; y \to Y$ as:

$$Y = \tau(M_1(y)) = \tau \left(\sum_{\alpha \in \mathbb{N}^n_m} y_\alpha A_\alpha \right).$$

It is easy to check that τ and σ are bijections and we can obtain the following lemma.

Lemma 2.1. *For any SDP matrix $X \in \Phi$, if $\bar{X} = \tau(X)$, then $\bar{X}$ is positive semidefinite and rank$(\bar{X}) =$ rank(X). For any matrix $\bar{X}$, it holds $\tau^{-1}(\bar{X})$ is semidefinite and rank$(\bar{X}) =$ rank$(\tau^{-1}(\bar{X}))$.*

Proof. A further examination the definition of τ shows that its inverse is the map that deletes some specified columns and rows of the given matrix. Specifically, X is the matrix that $\bar{X}$ deletes its specified columns and rows. Consequently, the positive semidefiniteness property and the rank of the two matrices are equivalent. □

Theorem 2.2. *Let y be an optimal solution of* (2.9)*. Then $Y = \sigma(y)$ is an optimal solution of* (2.14)*. Conversely, if Y is an optimal solution of* (2.14)*, then $y = \sigma^{-1}(Y)$ is an optimal solution of* (2.9)*.*

Proof. Due to the optimality of y, we have $M_1(y) \succeq 0$ and $\langle g, y \rangle = 1$. Lemma 2.1 implies that $Y = \sigma(y) = \tau(M_1(y))$ is positive semidefinite. It can be proved that the following relationship holds

$$\langle g, y \rangle = \sum_{\alpha \in \mathbb{N}^n_d} \frac{d!}{\prod_{j=1}^n \alpha_j!} y_{(2\alpha_1, \ldots, 2\alpha_n)} = \sum_{i=1}^{n^d} Y_{i,i} = \mathrm{tr}(Y). \tag{2.18}$$

Hence, Y is a feasible solution of (2.14). It also holds:

$$\langle F, Y \rangle = \sum_{\alpha \in \mathbb{N}^n_m} \langle F, y_\alpha B_\alpha \rangle = \sum_{\alpha \in \mathbb{N}^n_m} c_\alpha y_\alpha = \langle c, y \rangle. \tag{2.19}$$

If Y is not optimal to (2.14), there exists another $\tilde{Y}$ such that $\left\langle F, \tilde{Y} \right\rangle > \langle F, Y \rangle$. Then, based on the two equations (2.18) and (2.19), we have $\tilde{y} = \sigma^{-1}(\tilde{Y})$ is a feasible solution of (2.9) and $\langle f, \tilde{y} \rangle > \langle f, y \rangle$. This is a contradiction since y is an optimal solution of (2.9). Therefore, Y is an optimal solution of (2.14). The other part, namely, the optimality of $y = \sigma^{-1}(Y)$, can be proved in a similar fashion. □

3 The BEC Problem

In the BEC problem, the energy functional is defined as

$$E(\phi) = \int_{\mathbb{R}^d} \left[\frac{1}{2} |\nabla \phi(\mathbf{x})|^2 + V(\mathbf{x}) |\phi(\mathbf{x})|^2 + \frac{\beta}{2} |\phi(\mathbf{x})|^4 - \Omega \bar{\phi}(\mathbf{x}) L_z \phi(\mathbf{x}) \right] d\mathbf{x}, \tag{3.1}$$

where $\mathbf{x} = (x, y, z)^\top \in \mathbb{R}^3$ is the spatial coordinate vector, $\bar{f}$ denotes the complex conjugate of f, $L_z = -i(x\partial_y - y\partial_x)$, $V(x)$ is an external trapping potential, and $m, \hbar, N, \Omega, U_0$ are all constants. The ground state of a BEC is usually defined as the minimizer of the following nonconvex minimization problem

$$\phi_g = \arg\min_{\phi \in S} \quad E(\phi), \tag{3.2}$$

where the spherical constraint S is defined as

$$S = \left\{ \phi \mid E(\phi) < \infty, \int_{\mathbb{R}^d} |\phi(\mathbf{x})|^2 d\mathbf{x} = 1 \right\}. \tag{3.3}$$

Problem 3.2 is also related the Gross-Pitaevskii equation (GPE) in three dimensions (3D) [15] as

$$i\hbar \frac{\partial \psi(\mathbf{x}, t)}{\partial t} = \left(-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{x}) + N U_0 |\psi(\mathbf{x}, t)|^2 - \Omega L_z \right) \psi(\mathbf{x}, t), \tag{3.4}$$

where t is time.

The energy functional (3.1) and constraint (3.3) in the infinite dimensional optimization problem (3.2) can be discretized by methods such as the finite difference, sine pseudospectral and fourier pseudospectral methods. After a suitable discretization, problem (3.2) becomes a homogeneous quadratic and quartic polynomial with a single spherical constraint (HQQS) minimization problem:

$$\begin{aligned} \min_x \quad & f(x) := \frac{1}{2} x^\top A x + \frac{\beta}{2} \sum_{i=1}^n x_i^4 \\ \text{s. t.} \quad & \|x\|_2 = 1, \end{aligned} \tag{3.5}$$

where $\beta > 0$, and A is an n by n symmetric real or complex matrix. In the setting of BEC, A can be a Hermitian indefinite matrix. Considering to the structure and multiplying the quadratic term of the objective function by $x^\top x$, we convert the HQQS problem into the following equivalent form:

$$\begin{cases} \min\limits_x & f(x) = \frac{1}{2} x^\top A x x^\top x + \frac{\beta}{2} \sum_{i=1}^n x_i^4 \\ \text{s.t.} & \|x\|_2 = 1. \end{cases} \tag{3.6}$$

Clearly, problem (3.6) can be seen as the best rank-1 tensor approximation to a 4th-order symmetric tensor $\mathcal{F}$. Specifically, the entries of the tensor $\mathcal{F}$ are

$$\mathcal{F}_{\pi(i,j,k,l)} = \begin{cases} a_{kl}/4, & i = j = k \neq l, \\ a_{kl}/12, & i = j, i \neq k, i \neq l, k \neq l, \\ (a_{ii} + a_{kk})/12, & i = j \neq k = l, \\ a_{ii}/2 + \beta/4, & i = j = k = l, \\ 0, & \text{others}. \end{cases} \tag{3.7}$$

Consequently, the BEC problem can be solved by algorithms on finding the best rank-1 tensor approximations.

3.1 NP-hardness of HQQS

We prove in this subsection that HQQS is NP-complete by showing that the partition problem is a special instance of HQQS. First, we review the NP-completeness of the partition problem [25].

Proposition 3.1. *Given a set $\Omega := \{a_1, ..., a_n\}$ with cardinality n, checking whether there exists a equal partition of Ω is NP-complete.*

The next theorem establish the connection between the partition problem and HQQS.

Theorem 3.2. *Given a set $\Omega := \{a_1, ..., a_n\}$, the corresponding partition problem is an instance of HQQS.*

Proof. By letting $\theta_i = \frac{\sum_{j\neq i}^{n} a_j^4}{(\sum_{k=1}^{n} a_k^2)^2}$, $\gamma_i = \left(\frac{a_i^2}{(\sum_{k=1}^{n} a_k^2)} - 1\right)^2$ $(i = 1, 2, \cdots, n)$, we construct the following HQQS problem with

$$A = \begin{pmatrix} \theta_1 + \gamma_1 + 1 & 1 & \cdots & 1 \\ 1 & \theta_2 + \gamma_2 + 1 & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \cdots & \theta_n + \gamma_n + 1 \end{pmatrix}$$

and $\beta = 1$. Then, we have

$$\begin{aligned} 2f(x) &= x^{\mathrm{T}}Ax + \beta\sum_{i=1}^{n} x_i^4 = x^{\mathrm{T}}Ax + \sum_{i=1}^{n} x_i^4 \\ &= \sum_{i=1}^{n} (\theta_i + \gamma_i)\, x_i^2 + \left(\sum_{i=1}^{n} x_i\right)^2 + \sum_{i=1}^{n} x_i^4 \\ &= \sum_{i=1}^{n} \left(\frac{\sum_{j=1}^{n} a_j^4}{(\sum_{k=1}^{n} a_k^2)^2} + 1\right) x_i^2 - \frac{2\sum_{i=1}^{n} a_i^2 x_i^2}{\sum_{k=1}^{n} a_k^2} + \left(\sum_{i=1}^{n} x_i\right)^2 + \sum_{i=1}^{n} x_i^4 \\ &= 1 + \sum_{i=1}^{n}\left(x_i^2 - \frac{a_i^2}{\sum_{k=1}^{n} a_k^2}\right)^2 + \left(\sum_{i=1}^{n} x_i\right)^2 \\ &\geqslant 1. \end{aligned} \tag{3.8}$$

The last equality uses the spherical constraint. The equality holds in the last inequality, only if

$$\begin{aligned} x_i &= \pm a_i / \sqrt{\sum_{k=1}^{n} a_k^2}, \\ 0 &= \sum_{i=1}^{n} x_i, \end{aligned} \tag{3.9}$$

holds at the same time. They actually imply that there exists a partition of Ω. On the other hand, if (3.9) holds, the spherical constraint is satisfied. Therefore, this completes the proof. □

3.2 Quadratic SDP Relaxation To HQQS

Since the BEC problem (3.5) can be formulated as a 4th-order symmetric tensor (3.7), the two SDP relaxations in section 2 can be applied directly. The main limitation of using these two approaches to solve BEC problems is that the scales of these two SDP relaxations grow exponentially with the increase of the size of the original problem (3.5). Hence, we propose an SDP relaxation based on the specific structure of (3.5) with both deterministic and randomized rounding procedures in this section. Without loss of generality, in the remaining of this subsection, we assume matrix A is positive semidefinite. Otherwise, we can find a sufficiently large $\gamma > 0$ such that $A + \gamma I \succeq 0$, and consider

$$\begin{aligned} \min_x \quad & f(x) := \frac{1}{2} x^\top (A + \gamma I) x + \frac{\beta}{2} \sum_{i=1}^n x_i^4 \\ \text{s. t.} \quad & \|x\|_2 = 1, \end{aligned} \tag{3.10}$$

Due to the constraint $\|x\|_2 = 1$, it is easy to see that (3.10) shares the same optimal solution with HQQS problem (3.5).

3.2.1 A Deterministic Algorithm

Introducing a variable $X = xx^\top$, the HQQS problem is equivalent to

$$\begin{cases} \min\limits_X & \frac{1}{2} \langle A, X \rangle + \frac{\beta}{2} \sum_{i=1}^n X_{ii}^2 \\ \text{s. t.} & X \succeq 0, \quad \text{tr}(X) = 1, \quad \text{rank}(X) = 1. \end{cases} \tag{3.11}$$

By ignoring the rank-one constraint, we obtain a convex quadratic SDP relaxation

$$\begin{cases} \min\limits_X & \frac{1}{2} \langle A, X \rangle + \frac{\beta}{2} \sum_{i=1}^n X_{ii}^2 \\ \text{s.t.} & \text{tr}(X) = 1, \quad X \succeq 0. \end{cases} \tag{3.12}$$

Let X^* be a solution to (3.12) and $\text{rank}(X^*) = r$. It follows from [13] that there exists r vectors $x^1, x^2, \cdots, x^r$ such that $X^* = \sum_{k=1}^r x^k (x^k)^\top$ and

$$\text{tr}(x^k (x^k)^\top) = (x^k)^\top x^k = \text{tr}(X^*)/r = 1/r, \ \forall\, k = 1, \ldots, r. \tag{3.13}$$

Then we compute

$$\hat{x} = \arg \min_{x^k, k=1,\ldots,r} \frac{1}{2} (x^k)^\top A x^k + \frac{\beta}{2} \sum_{i=1}^n (x_i^k)^4 \quad \text{and} \quad x^* = \sqrt{r} \hat{x}. \tag{3.14}$$

Obviously $(x^*)^\top x^* = r(\hat{x})^\top \hat{x} = 1$ which means that x^* is feasible to the HQQS problem. The quality of the approximate solution x^* is summarized in the next theorem.

Theorem 3.3. *Suppose that A is positive definite. Let X^* be an optimal of (3.12) with rank$(X^*) = r$ and x^* be constructed based on (3.13) and (3.14). Then x^* is an approximate solution to the HQQS problem with an approximation ratio $r \leqslant n$.*

Proof. Since A is positive definite, it follows from the definition of $\hat{x}$ that

$$\begin{aligned} \frac{1}{2} (x^*)^\top A x^* + \frac{\beta}{2} \sum_{i=1}^n (x_i^*)^4 &= \frac{r}{2} (\hat{x})^\top A \hat{x} + \frac{\beta\, r^2}{2} \sum_{i=1}^n (\hat{x}_i)^4 \\ &\leqslant \frac{r^2}{2} (\hat{x})^\top A \hat{x} + \frac{\beta\, r^2}{2} \sum_{i=1}^n (\hat{x}_i)^4 \\ &\leqslant r \sum_{k=1}^r \left(\frac{1}{2} (x^k)^\top A x^k + \frac{\beta}{2} \sum_{i=1}^n (x_i^k)^4 \right) \\ &= r \left(\frac{1}{2} \langle A, X^* \rangle + \frac{\beta}{2} \sum_{k=1}^r \sum_{i=1}^n (x_i^k)^4 \right) \end{aligned}$$

$$\leqslant \; r\left(\frac{1}{2}\langle A, X^*\rangle + \frac{\beta}{2}\sum_{i=1}^n\left(\sum_{k=1}^r (x_i^k)^2\right)^2\right)$$
$$= \; r\left(\frac{1}{2}\langle A, X^*\rangle + \frac{\beta}{2}\sum_{i=1}^n (X_{ii}^*)^2\right) \leqslant r\, f_{\min}(HQQS),$$

where $f_{\min}(HQQS)$ is the objective function value of the global optimal solution of (3.5). The last inequality holds because (3.12) is relaxation of (3.11). This completes the proof. □

3.2.2 A Randomized Algorithm

We now consider the same SDP relaxation (3.12), and let X^* be its global minimizer. Different to the previous discussion, our goal is to recover a feasible solution of problem HQQS (3.5) with some quality guarantee through a randomized procedure. In particular, recall that when ξ is a random vector drawn from a Gaussian distribution $\mathcal{N}(0, X^*)$, we have that $\mathsf{E}[\xi^\top \xi] = \mathrm{tr}(X^*) = 1$ and (see for example [11])

$$\begin{aligned} \mathsf{E}\left[f(\xi)\right] = \mathsf{E}\left[\frac{1}{2}\xi^\top A\xi + \frac{\beta}{2}\sum_{i=1}^n \xi_i^4\right] &= \frac{1}{2}\langle A, X^*\rangle + \frac{3\,\beta}{2}\sum_{i=1}^n (X_{ii}^*)^2 \\ &\leqslant 3\left(\frac{1}{2}\langle A, X^*\rangle + \frac{\beta}{2}\sum_{i=1}^n (X_{ii}^*)^2\right) \\ &\leqslant 3\left(\frac{1}{2}(x^*)^\top A x^* + \frac{\beta}{2}\sum_{i=1}^n (x_i^*)^4\right) = 3f(x^*), \end{aligned}$$

where x^* is an optimal solution to problem HQQS (3.5). Based on the above observations, we are interested in the following event:

$$\left\{f(\xi) < \alpha\, \mathsf{E}[f(\xi)],\; \xi^\top\xi \geqslant \mathrm{tr}(X^*) \geqslant 1\right\}.$$

This is because once the above event does occur, we can construct $\hat{x} = \xi/\|\xi\|_2$ and obtain

$$\begin{aligned} f(\hat{x}) = \frac{1}{2\,\|\xi\|_2^2}\xi^\top A\xi + \frac{\beta}{2\,\|\xi\|_2^4}\sum_{i=1}^n \xi_i^4 &\leqslant \frac{1}{2}\xi^\top A\xi + \frac{\beta}{2}\sum_{i=1}^n \xi_i^4 \\ &\leqslant \alpha\left(\frac{1}{2}\langle A, X^*\rangle + \frac{3\,\beta}{2}\sum_{i=1}^n (X_{ii}^*)^2\right) \\ &\leqslant 3\alpha\, f(x^*). \end{aligned}$$

Thus $\hat{x}$ is an approximate solution to problem HQQS with approximation ratio 3α. Therefore, the key is to estimate how likely the above event happens. To this end, we first quote a useful result from [26].

Lemma 3.4. *Let ξ be a random variable with bounded fourth order moment. Suppose that $\mathsf{E}[(\xi - \mathsf{E}(\xi))^4] \leqslant \tau\, \mathsf{Var}^2(\xi)$, for some $\tau > 0$. Then*

$$\mathsf{Prob}\{\xi \geqslant \mathsf{E}(\xi)\} \geqslant 0.25/\tau \quad \textit{and} \quad \mathsf{Prob}\{\xi \leqslant \mathsf{E}(\xi)\} \geqslant 0.25/\tau.$$

The key step of our argument is based on the following lemma.

Lemma 3.5. *Let $Q \in S_+^{n\times n}$. Suppose $\eta \in \mathbb{R}^n$ is a random vector generated from Gaussian distribution $\mathcal{N}(0, I)$. Then,*

$$\mathsf{Prob}\left(\eta^\top Q\eta < \mathsf{E}[\eta^\top Q\eta]\right) \leqslant 1 - \theta$$

where $\theta := 1/960$.

Proof. Recall that for a standard Gaussian $\zeta \sim \mathcal{N}(0,1)$, its even order moments can be calculated explicitly as

$$\mathsf{E}[\zeta^2] = 1,\ \mathsf{E}[\zeta^4] = 3,\ \mathsf{E}[\zeta^6] = 15,\ \mathsf{E}[\zeta^8] = 105.$$

To apply Lemma 3.4, we treat $\eta^\top Q\eta$ as a random variable and compute its fourth order central moment as well as the variance. To this end, we notice that

$$\begin{aligned}
\mathsf{Var}[\eta^\top Q\eta] &= \mathsf{E}[(\eta^\top Q\eta)^2] - \mathsf{E}[\eta^\top Q\eta]^2 \\
&= \mathsf{E}[(\eta^\top Q\eta)^2] - \big(\mathrm{tr}(Q)\big)^2 \\
&= \mathsf{E}\left[\sum_{i=1}^n Q_{ii}^2\eta_i^4 + 2\sum_{i\neq j} Q_{ij}^2\eta_i^2\eta_j^2 + \sum_{i\neq j} Q_{ii}Q_{jj}\eta_i^2\eta_j^2\right] - (\sum_{i=1}^n Q_{ii})^2 \\
&= 3\sum_{i=1}^n Q_{ii}^2 + 2\sum_{i\neq j} Q_{ij}^2 + \sum_{i\neq j} Q_{ii}Q_{jj} - (\sum_{i=1}^n Q_{ii})^2 \\
&= 2\left(\sum_{i=1}^n Q_{ii}^2 + \sum_{i\neq j} Q_{ij}^2\right).
\end{aligned}$$

On the other hand,

$$\begin{aligned}
\mathsf{E}[(\eta^\top Q\eta - \mathrm{tr}(Q))^4] &= \mathsf{E}[(\sum_{i=1}^n Q_{ii}(\eta_i^2 - 1) + \sum_{i\neq j} Q_{ij}^2\eta_i\eta_j)^4] \\
&\leqslant 16\left(\mathsf{E}\big[\big(\sum_{i=1}^n Q_{ii}(\eta_i^2-1)\big)^4\big] + \mathsf{E}\big[\big(\sum_{i\neq j} Q_{ij}^2\eta_i\eta_j\big)^4\big]\right).
\end{aligned}$$

Moreover, a straight forward computation implies that

$$\begin{aligned}
\mathsf{E}\big[\big(\sum_{i=1}^n Q_{ii}(\eta_i^2-1)\big)^4\big] &= \mathsf{E}[(\sum_{i=1}^n Q_{ii}^4(\eta_i^2-1)^4] + 3\mathsf{E}[\sum_{i\neq j} Q_{ii}^2 Q_{jj}^2(\eta_i^2-1)^2(\eta_j^2-1)^2] \\
&\leqslant 60\sum_{i=1}^n Q_{ii}^4 + 12\sum_{i\neq j} Q_{ii}^2 Q_{jj}^2 \\
&\leqslant 60\left(\sum_{i=1}^n Q_{ii}^2\right)^2.
\end{aligned}$$

Similarly, we can show that

$$\mathsf{E}\big[\big(\sum_{i\neq j} Q_{ij}^2\eta_i\eta_j\big)^4\big] \leqslant 9\left(\sum_{i\neq j} Q_{ij}^2\right)^2.$$

Combining the above two equalities yields that

$$\mathsf{E}[(\eta^\top Q\eta - \mathrm{tr}(Q))^4] \leqslant 16\left(60\left(\sum_{i=1}^n Q_{ii}^2\right)^2 + 9\left(\sum_{i\neq j} Q_{ij}^2\right)^2\right) \leqslant 240\,\mathsf{Var}[\eta^\top Q\eta]^2.$$

Finally, invoking Lemma 3.4 gives that

$$\mathsf{Prob}\left(\eta^\top Q\eta \geqslant \mathsf{E}[\eta^\top Q\eta]\right) \geqslant 1/(240 * 4),$$

which in term implies the desired inequality. □

When ξ is drawn from $\mathcal{N}(0,\hat{X})$, we can let $\eta \sim \mathcal{N}(0,I)$ such that $\xi = X^{*1/2}\eta$. Then applying Lemma 3.5 with $Q = X^*$ yields that

$$\mathsf{Prob}\left(\xi^\top \xi < \mathrm{tr}(X^*)\right) = \mathsf{Prob}\left(\eta^\top \hat{X}\eta < \mathsf{E}[\eta^\top \hat{X}\eta]\right) \leqslant 1-\theta.$$

Moreover, we note that $f(\xi) \geqslant 0$ and by Markov's inequality

$$\mathsf{Prob}\left(f(\xi) \geqslant \rho \mathsf{E}[f(\xi)]\right) \leqslant 1/\rho^2.$$

Therefore, by union bound and letting $\rho = \sqrt{2/\theta}$, we have that

$$\begin{aligned} & \mathsf{Prob}\left(f(\xi) < \sqrt{2/\theta}\ \mathsf{E}[f(\xi)],\ \xi^\top\xi \geqslant \mathrm{tr}(X^*) \geqslant 1\right) \\ \geqslant\ & 1 - \mathsf{Prob}\big(f(\xi) \geqslant \sqrt{2/\theta}\ \mathsf{E}[f(\xi)]\big) - \mathsf{Prob}\big(\xi^\top\xi < \mathrm{tr}(X^*)\big) \\ =\ & 1 - \theta/2 - (1-\theta) \\ \geqslant\ & \theta/2 > 0. \end{aligned}$$

Combining the above discussions leads to the following theorem.

Theorem 3.6. *Suppose that A is positive definite, X^* is a solution to* (3.12) *and random variable ξ is drawn from $\mathcal{N}(0,X^*)$. Construct $\hat{x} = \xi/\|\xi\|_2$, then we have*

$$\mathsf{Prob}\left(f(\hat{x}) \leqslant 3\sqrt{2/\theta}\ f_{\min}(HQQS)\right) \geqslant \theta/2$$

with $\theta := 1/960$.

As far as we know, the best approximation ratio for quartic polynomial optimization with a single sphere constraint is $O(n/\ln n)$ in [18,19], and the ratio under consideration is relative ratio. The merit of our approximation scheme is that both approximation ratios obtained by our two algorithms are absolute ones. In particular, the ratio associated with the deterministic algorithm depends on the rank of the optimal solution of (3.12). Normally, we only know that dimension n is a trivial upper bound of this rank. However, further information is not available in most cases. On the other hand, the randomized algorithm provides us a constant approximation ratio, which is independent of the problem dimension n. Moreover, the probability of obtaining a solution with the assured quality is dimensional free as well. To our best knowledge, this is the first constant approximation ratio for polynomial optimization, although this result relies on the special structure of our problem.

3.3 A Feasible Method For Solving the Quadratic SDP Relaxations

Note that (3.12) is a convex quadratic SDP. Many algorithms such as the alternating direction method of multipliers can be applied to solve them. In this subsection, we briefly describe the feasible gradient method proposed in [14].

Suppose that the solution $\bar{X}$ of (3.12) is rank p. Then $\bar{X}$ can be decomposed as $\bar{X} = V^\top V$ with $V = [V_1,\cdots,V_n] \in \mathbb{R}^{p\times n}$ according to [14, 24]. Consequently, we convert (3.12) into an equivalent problem

$$\max_{V=[V_1,\cdots,V_n]} f(V) := \frac{1}{2}\left\langle A, V^\top V\right\rangle + \frac{\beta}{2}\|\mathrm{diag}(V^\top V)\|_2^2, \quad \text{s. t. } \|V\|_F = 1, \quad i = 1,\cdots,n, \tag{3.15}$$

where $\mathrm{diag}(V^\top V)$ is the diagonals of $V^\top V$. Although (3.15) is again a nonconvex problem, it can be solved by the feasible gradient method in [14]. In fact, it has been a common practice to solve a nonconvex counterpart of the SDP relaxations when their size are huge.

We next briefly introduce the feasible gradient method. Let $G = \nabla f(V)$ denote the gradient of $f(V)$. A simple calculation yields:

$$G = VA + 2\beta V \mathrm{diag}(v),$$

where $v = [\|V_1\|^2, \|V_2\|^2, \cdots, \|V_n\|^2]$ and $\mathrm{diag}(v)$ is the diagonal matrix generated by v. Then the update scheme of the feasible gradient method is

$$Y(\tau) := V - \tau(GV^\top - VG^\top)(V + Y(\tau)), \tag{3.16}$$

where τ is the step size. The spherical constraint is preserved, i.e., $\|Y(\tau)\|_F = 1$, for any τ. The convergence of the method can be fast when a nonmonotone curvilinear search with the Barzilar-Borwein (BB) step size is used. Starting from an initial point $V^{(0)}$ and a step size τ^0 and setting $C^{(0)} = f(V^{(0)})$ and $Q^{(0)} = 1$, the new points are generated iteratively in the form $V^{(k+1)} := Y^{(k)}(\tau^{(k)})$ with $\tau^{(k)} = \tau\delta^m$, where τ is a BB step size. Here, m is the smallest nonnegative integer satisfying the descent condition

$$f(Y^{(k)}(\tau^{(k)})) \leqslant C^{(k)} - \rho\tau^{(k)}\|(G(V^{(k)})^\top - (V^{(k)})^\top G)V^{(k)}\|^2, \tag{3.17}$$

where each reference value $C^{(k+1)}$ is taken to be the convex combination of $C^{(k)}$ and $f(V^{(k+1)})$ as $C^{(k+1)} = (\eta Q^{(k)}C^{(k)} + f(V^{(k+1)}))/Q^{(k+1)}$ and $Q^{(k+1)} = \eta Q^{(k)} + 1$. A outline of the method is described in Algorithm 1.

Algorithm 1: A feasible gradient method

Given $V^{(0)}$, set $\tau, \rho, \eta \in (0, 1)$, $k = 0$.
while *stopping conditions are not met* **do**
    Compute $V^{(k+1)} \leftarrow Y(\tau\delta^m)$, where m is the smallest nonnegative integer satisfying the descent condition defined by (3.17).
    Set $Q^{(k+1)} \leftarrow \eta Q^{(k)} + 1$ and $C^{(k+1)} \leftarrow (\eta Q^{(k)}C^{(k)} + f(V^{(k+1)}))/Q^{(k+1)}$.
    Compute a BB step size τ.
    Set $k \leftarrow k + 1$.

4 Numerical Results

In this section, we present numerical results on the semidefinite relaxations on best rank-1 tensor approximation and the BEC problem. All of our numerical experiments are preformed on a workstation with two twelve-core Intel Xeon E5-2697 CPUs and 128GB of memory running Ubuntu 12.04 and MATLAB 2013b.

4.1 Verification of the Equivalence between the two SDP Approaches [7] and [8]

In this subsection, we report numerical results on solving the SDP relaxations (2.9) and (2.14) using different algorithms, including an interior point method SDPT3[1)] , the alternating direction method of multipliers (ADMM), the commercial software MOSEK[2)] and a semi-smooth Newton conjugate gradient method SDPNAL[3)] . For simplicity of presentation, the former SDP relaxation is denoted by NW and the latter is written as JMZ. The default parameters are used in each algorithm. We report the cpu time measured in seconds (, the optimal value of (2.14) denoted by λ and the residual $\|\mathcal{F} - \lambda \cdot x^{\otimes m}\|$ between the computed solution $\lambda \cdot x^{\otimes m}$ and the given tensor $\mathcal{F}$. For a given matrix A, its numerical rank is set to be the smallest r such that $\sigma_{r+1}/\sigma_r < 10^{-6}$, where $\sigma_1 \geqslant \sigma_2 \geqslant \cdots \geqslant \sigma_t > 0$ are the singular values of A.

Example 4.1 (Example 3.4 in [7])**.** Consider a tensor $\mathcal{F} \in S^{3^4}$ with entries:

$$\begin{aligned}
&\mathcal{F}_{1111} = 0.2883, && \mathcal{F}_{1112} = -0.0031, && \mathcal{F}_{1113} = 0.1973, && \mathcal{F}_{1122} = -0.2485, && \mathcal{F}_{1123} = -0.2939,\\
&\mathcal{F}_{1133} = 0.3847, && \mathcal{F}_{1222} = 0.2972, && \mathcal{F}_{1223} = 0.1862, && \mathcal{F}_{1233} = 0.0919, && \mathcal{F}_{1333} = -0.3619,\\
&\mathcal{F}_{2222} = 0.1241, && \mathcal{F}_{2223} = -0.3420, && \mathcal{F}_{2233} = 0.2127, && \mathcal{F}_{2333} = 0.2727, && \mathcal{F}_{3333} = -0.3054.
\end{aligned}$$

1) Downloadable from `http://www.math.nus.edu.sg/~mattohkc`
2) Downloadable from `https://www.mosek.com/`
3) Downloadable from `http://www.math.nus.edu.sg/~mattohkc`

We use SDPNAL to solve both SDPs NW and JMZ. They yield the same best rank-1 approximations of $\mathcal{F}$ with $\lambda = -1.0954$ and 1.9683 as defined in [7].

Example 4.2 (Example 3.6 in [7])**.** Consider a tensor $\mathcal{F} \in S^{n^4}$ with entries:

$$\mathcal{F}_{i_1\cdots i_4} = \arctan\left((-1)^{i_1}\frac{i_1}{n}\right) + \cdots + \arctan\left((-1)^{i_4}\frac{i_4}{n}\right)$$

by varying the values of n from 10 to 30. We use SDPNAL to solve both SDPs NW and JMZ. They return rank one solutions which are the best rank-1 approximation. A summary of numerical results are presented in Table 1. This table shows that NW is more efficient because its problem size is smaller.

n	time		λ		residual	
	NW	JMZ	NW	JMZ	NW	JMZ
10	1.8920	2.1132	77.0689	77.0689	72.8350	72.8350
15	5.0124	8.0642	-165.0695	-165.0695	164.6400	164.6400
20	14.8892	28.3321	282.9708	282.9708	295.9706	295.9706
25	7.2067	195.8824	-435.3512	-435.3512	463.0760	463.0760
30	14.4721	574.4781	617.5361	617.5361	669.7284	669.7284

Table 1 Computational results on tensor $\mathcal{F}_{i_1\cdots i_4} = \arctan\left((-1)^{i_1}\frac{i_1}{n}\right) + \cdots + \arctan\left((-1)^{i_4}\frac{i_4}{n}\right)$

Example 4.3 (Example 3.10 in [7])**.** Consider a tensor $\mathcal{F} \in S^{n^4}$ with entries:

$$\mathcal{F}_{i_1\cdots i_4} = \sin(i_1 + \cdots + i_4)$$

by varying n from 10 to 30. We still apply SDPNAL to solve both SDPs. All the returned matrices are rank one. The detailed numerical results are reported in Table 2. This table again shows that NW is more efficient because its problem size is smaller.

n	time		λ		residual	
	NW	JMZ	NW	JMZ	NW	JMZ
10	0.7699	1.0121	-27.2654	-27.2654	65.2419	65.2419
15	4.9850	8.4545	61.4169	61.4169	146.7665	146.7665
25	10.1289	72.0134	158.2156	158.2155	412.6504	412.6504
30	38.1121	254.3728	-241.6526	-241.6526	588.7309	588.7309

Table 2 Computational results on tensor $\mathcal{F}_{i_1\cdots i_4} = \sin(i_1 + \cdots + i_4)$

Example 4.4. We generate five random examples for $n = 10$ and 12 similar to [8]. The performance from different solvers SDPT3, ADMM, MOSEK and SDPNAL are reported in Table 3. We can see that SDPNAL is the most efficient solver.

4.2 Numerical comparisons on the BEC Problem

In this subsection, we present numerical results on one dimensional BEC problems [15].

Example 4.5. Consider a BEC problem with $d = 1, V(x) = \frac{1}{2}x^2$ and $\beta = 400$. The problems are discretized by the finite difference scheme on a domain $U = (-16, 16)$ with different mesh sizes $h =$

Instance	time				λ			
	SDPT3	ADMM	MOSEK	SDPNAL	SDPT3	ADMM	MOSEK	SDPNAL
Dimension $n = 10$								
1	18.3108	5.4023	20.2667	1.9938	4.8708	4.8708	4.8708	4.8708
2	18.7813	5.0224	18.3224	1.4156	4.4324	4.4324	4.4324	4.4324
3	23.2172	10.7752	19.9949	1.9375	4.6236	4.6237	4.6237	4.6236
4	14.0992	10.8524	21.6577	1.8614	4.6507	4.6508	4.6507	4.6507
5	15.8869	13.0126	18.8525	1.9756	4.5414	4.5414	4.5414	4.5414
Dimension $n = 12$								
1	97.8172	10.3173	75.3220	2.1984	5.2555	5.2556	5.2556	5.2556
2	80.2766	10.7515	86.9155	2.7042	4.7151	4.7151	4.7151	4.7151
3	79.8950	10.9313	86.0055	1.8049	5.4132	5.4132	5.4132	5.4132
4	69.6030	12.3825	82.8964	1.9321	5.5616	5.5615	5.5615	5.5615
5	69.2047	13.0897	81.4128	2.3453	5.6417	5.6417	5.6417	5.6417

Table 3 Comparisons between different algorithms

$2, 1, \frac{1}{2}, \frac{1}{4}, \frac{1}{6}, \frac{1}{8}$. We first compare solving these problems as the best rank-1 tensor approximation. A summary of numerical results are presented in Table 4.

We next use the regularized Newton method in [15], denoted by RN, to solve the original BEC problem and the feasible gradient method with default parameters to solve the quadratic SDP (3.12). The deterministic and randomized versions are denoted by SDR1 and SDR2, respectively. We report the cpu time measured in seconds, the objective function value corresponding to the original BEC problem denoted by λ, the rank of the SDR1 and SDR2 solutions and the ratio is between λ and the best objective function value for SDR1 and SDR2. Since SDR2 is a randomized algorithm, we repeat 50 random examples and report the best λ but present the maximum, mean and minimum of the ratios. The numerical results are reported in Table 5.

From the Table 5, we can see that the objective function value obtained by SDR1 is almost the same as RN. The ratios of SDR2 show that the best objective function values do not exceed the $\sqrt{(2/\theta)}$ times of the function value of SDR2. Although the computational costs of SDR1 and SDR2 are more expensive than that of RN, they can provide certain theoretical guarantee on the solution qualities.

Example 4.6. Consider a BEC problem with $d = 1, V(x) = \frac{1}{2}x^2 + 25\sin^2(\frac{\pi x}{4})$ and $\beta = 250$. We discretize the problem by the finite difference scheme on a domain $U = (-16, 16)$ with different mesh sizes $h = 2, 1, \frac{1}{2}, \frac{1}{4}, \frac{1}{6}, \frac{1}{8}$. A summary of numerical results of the best rank-1 tensor approximation is presented in Table 6. The computational results for the case $h = 1$ are not reported because SDPNAL encountered into numerical troubles and it did not solve the SDP generated by NW accurately. The comparison between RN, SDR1 and SDR2 are shown in Table 7.

Conclusions

Minimizing a polynomial function over a single sphere is an important but challenging problem. In this paper, we first compare recent two SDP relaxations in [7] and [8] for computing the best rank-one tensor approximation. Although the appearance of these two SDP relaxations look quite different, they are essentially equivalent. We then consider a specific example arising from Bose-Einstein condensates, whose

h	time		λ	
	NW	JMZ	NW	JMZ
2	5.5782	22.3343	21.3773	21.3773
1	110.7321	1483.9856	21.3592	21.3592
1/2	—	—	—	—
1/4	—	—	—	—
1/6	—	—	—	—
1/8	—	—	—	—

Table 4. Computational results on Example 4.5. "—" means that the computational time is more than 30 minutes.

h	time			λ			rank (ratio)	
	RN	SDR1	SDR2	RN	SDR1	SDR2	SDR1	SDR2
2	0.0070	0.0702	0.0736	21.3773	21.5434	22.5696	5(1.0077)	5(18.3641,4.9596,1.0558)
1	0.0105	0.0864	0.0860	21.3592	21.3896	21.5076	5(1.0014)	5(43.2324,5.9762,1.0069)
1/2	0.0115	0.1704	0.1895	21.3598	21.3858	21.7901	5(1.0012)	5(22.6133,4.8358,1.0201)
1/4	0.0120	0.1029	0.1876	21.3600	21.3886	21.5701	5(1.0013)	5(35.6182,5.8311,1.0098)
1/6	0.0148	0.1963	0.2083	21.3600	21.3952	21.7423	5(1.0016)	5(21.3470,4.6358,1.0179)
1/8	0.0181	0.4024	0.6933	21.3601	21.3786	21.4868	5(1.0009)	5(41.1597,6.3262,1.0059)

Table 5 Computational results of RN and quadratic SDPs on Example 4.5

objective function is a summation of a quadratic and quartic function. Since the two SDP relaxations for the best rank-1 tensor approximation usually are not suitable due to the large SDP matrix dimension, we propose a much smaller quadratic SDP relaxation. Then both deterministic and randomized rounding procedures are developed and approximation ratios between function values at the global minimum and the solution constructed from rounding procedures are provided. Although the computational costs of the SDP relaxations are usually more expensive, they can provide us a better understanding on finding the global optimal solutions.

References

1 P.-A. Absil, R. Mahony, and R. Sepulchre, *Optimization algorithms on matrix manifolds*, Princeton University Press, Princeton, NJ, 2008.

2 W. Bao, I.L. Chern, and Y. Zhang, *Efficient numerical methods for computing ground states of spin-1 Bose-Einstein condensates based on their characterizations*, J. Comput. Phys., 253 (2013), pp. 189–208.

3 W. Bao and H. Wang, *A mass and magnetization conservative and energy-diminishing numerical method for computing ground state of spin-1 Bose-Einstein condensates*, SIAM J. Numer. Anal., 45 (2007), pp. 2177–2200.

4 W. Bao and H. Wang, *Ground states and dynamics of spin-orbit-coupled Bose-Einstein condensates*, SIAM J. Appl. Math., 75 (2015), pp. 492-517.

5 W. Bao, Y. Cai and H. Wang, *Efficient numerical methods for computing ground states and dynamics of dipolar Bose-Einstein condensates*, J. Comput. Phys., 229 (2010), pp. 7874-7892.

6 I. Danaila and P. Kazemi, *A new Sobolev gradient method for direct minimization of the Gross-Pitaevskii energy with rotation*, SIAM J. Sci. Comput., 32 (2010), pp. 2447-2467.

h	time		λ	
	NW	JMZ	NW	JMZ
2	5.0423	26.0845	23.8977	23.8976
1/2	—	—	—	—
1/4	—	—	—	—
1/6	—	—	—	—
1/8	—	—	—	—

Table 6. Computational results on Example 4.6. "—" means that the computational time is more than 30 minutes.

h	time			λ			rank (ratio)	
	RN	SDR1	SDR2	RN	SDR1	SDR2	SDR1	SDR2
2	0.0220	0.0792	0.0816	23.8977	24.3978	24.7984	5(1.0209)	5(37.0336,6.0068,1.0377)
1	0.0283	0.0829	0.0869	26.0573	26.0932	27.3979	5(1.0014)	5(10.6342,3.0240,1.0514)
1/2	0.2025	0.0747	0.1614	26.0755	26.0865	26.4186	5(1.0004)	5(21.2076,5.3864,1.0132)
1/4	0.1523	0.0826	0.4497	26.0818	26.1140	26.9123	5(1.0012)	5(50.9194,4.9634,1.0318)
1/6	0.0418	0.0945	0.2976	26.0830	26.1078	26.6175	5(1.0009)	5(16.3740,3.96301.0215)
1/8	0.0523	0.1047	0.3095	26.0834	26.1119	27.8197	5(1.0011)	5(35.7704,6.1598,1.0666)

Table 7 Computational results of RN and quadratic SDPs on Example 4.6

7 J. Nie, L. Wang, *Semidefinite relaxations for best rank-1 tensor approximations.* SIAM J. Matrix Anal. Appl., 35 (2014), pp. 1155-1179.

8 B. Jiang, S. Ma, S. Zhang, *Tensor principal component analysis via convex optimization.* Math. Program. Ser. A. 150 (2015), pp. 423-457.

9 De Lathauwer L, De Moor B, Vandewalle J, *On the best rank-1 and rank-$(r_1, r_2, \cdots, r_n)$ approximation of higher-order tensors.* SIAM J. Matrix Anal. Appl., 21 (2000), pp. 1324-1342.

10 X. Zhang, C. Ling, L. Qi, *The best rank-1 approximation of a symmetric tensor and related spherical optimization problems.* SIAM J. Matrix Anal. Appl., 33 (2012), pp. 806-821.

11 W. Bar, and F. Dittrich, *Useful formula for moment computation of normal random variables with nonzero means*, Automatic Control, IEEE Transactions on, 16 (1971), pp. 263-265.

12 Z-Q. Luo, N.D. Sidiropoulos, P. Tseng, and S. Zhang, *Approximation bounds for quadratic optimization with homogeneous quadratic constraints*, SIAM J. Optim, 18 (2007), pp. 1-28,

13 J.F. Sturm and S. Zhang, *On Cones of Nonnegative Quadratic Functions*, Math. Oper. Res., 28 (2003), pp. 246-267,

14 Z. Wen and W. Yin, *A feasible method for optimization with orthogonality constraints*, Math. Program. Ser. A., 142 (2013), pp. 397-434.

15 X. Wu, Z. Wen and W. Bao, *A Regularized Newton Method for Computing Ground States of Bose-Einstein condensates*, arXiv preprint arXiv:1504.02891, 2015.

16 E. Kofidis and P. Regalia, *On the best rank-1 approximation of higher-order supersymmetric tensors.* SIAM J. Matrix Anal. Appl., 23 (2002), pp. 863-884.

17 S. Hu, Z. H. Huang and L. Qi, *Finding the extreme Z-eigenvalues of tensors via a sequential semidefinite programming method.* Numer. Linear Algebra Appl., 20 (2013), pp. 972-984.

18 Anthony M.-C. So, *Deterministic approximation algorithms for sphere constrained homogeneous polynomial optimization problems*, Math. Program. Ser. B, 129 (2011), pp. 357-382.

19 S. He, B. Jiang, Z. Li and S. Zhang, *Probability Bounds for Polynomial Functions in Random Variables*, Math. Oper. Res., 39 (2014), 889-907.

20 S. He, Z. Li, and S. Zhang, *Approximation algorithms for homogeneous polynomial optimization with quadratic constraints*, Math. Program. Ser. B, 125 (2010), pp. 353-383.

21 J. Nocedal and S.J. Wright, *Numerical Optimization, Springer Series in Operations Research and Financial Engineering*, Springer, New York, second ed., 2006.

22 Tamara G. Kolda and Jackson R. Mayo, *Shifted power method for computing tensor eigenpairs*, SIAM J. Matrix Anal. Appl., 32 (2011), pp. 1095-1124.

23 J. J. Hilling and A. Sudbery, *The geometric measure of multipartite entanglement and the singular values of a hypermatrix*, J. Math. Phys., 51 (2010): 072102

24 S. Burer and R. D. C. Monteiro, *A nonlinear programming algorithm for solving semidefinite programs via low-rank factorization*, Math. Program., 95 (2003), pp. 329-357.

25 Garey, M.R., and D.S. Johnson, *Computers and Intractability: A Guide to the Theory of NP-Completeness*, San Francisco, LA: Freeman, 1979.

26 S. He, Z.-Q. Luo, J. Nie, and S. Zhang, *Semidefinite relaxation bounds for indefinite homogeneous quadratic optimization*, SIAM J. Optim., 19 (2008), pp. 503-523.