

Minimum-Volume Enclosing Ellipsoids and Core Sets¹

P. KUMAR² AND E. A. YILDIRIM³

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Abstract. We study the problem of computing a $(1 + \epsilon)$ -approximation to the minimum-volume enclosing ellipsoid of a given point set $S = \{p^1, p^2, \dots, p^n\} \subseteq \mathbb{R}^d$. Based on a simple, initial volume approximation method, we propose a modification of the Khachiyan first-order algorithm. Our analysis leads to a slightly improved complexity bound of $O(nd^3/\epsilon)$ operations for $\epsilon \in (0, 1)$. As a byproduct, our algorithm returns a core set $\mathcal{X} \subseteq S$ with the property that the minimum-volume enclosing ellipsoid of \mathcal{X} provides a good approximation to that of S . Furthermore, the size of \mathcal{X} depends on only the dimension d and ϵ , but not on the number of points n . In particular, our results imply that $|\mathcal{X}| = O(d^2/\epsilon)$ for $\epsilon \in (0, 1)$.

Key Words. Löwner ellipsoids, core sets, approximation algorithms.

1. Introduction

We study the problem of computing the minimum-volume enclosing ellipsoid (MVEE) of a given point set $S = \{p^1, \dots, p^n\} \subseteq \mathbb{R}^d$, denoted by $\text{MVEE}(S)$, also known as the Löwner ellipsoid for S . Minimum-volume enclosing ellipsoids play an important role in several diverse applications such as optimal design (Refs. 1–2), computational geometry (Refs. 3–5), convex optimization (Ref. 6), computer graphics (Refs. 7–8), pattern recognition (Ref. 9), and statistics (Ref. 10). Variations of this problem

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²Assistant Professor, Computer Science Department, Florida State University, Tallahassee, Florida. This author was supported in part by NSF through Grant CCR-0098172.

³Assistant Professor, Department of Applied Mathematics and Statistics, Stony Brook University, Stony Brook, New York. This author was supported in part by NSF through CAREER Grant DMI-0237415.

such as the MVEE with outliers (Ref. 11) have many other applications (Refs. 12–14).

A full-dimensional ellipsoid $\mathcal{E}_{Q,c}$ in \mathbb{R}^d is specified by a $d \times d$ symmetric positive-definite matrix Q and a center $c \in \mathbb{R}^d$ and is defined as

$$\mathcal{E}_{Q,c} = \{x \in \mathbb{R}^d : (x - c)^T Q (x - c) \leq 1\}. \quad (1)$$

The volume of an ellipsoid $\mathcal{E}_{Q,c}$, denoted by $\text{vol } \mathcal{E}_{Q,c}$, is given by

$$\text{vol } \mathcal{E}_{Q,c} = \eta \det Q^{-1/2},$$

where η is the volume of the unit ball in \mathbb{R}^d (Ref. 6).

In Ref. 15, F. John proved that the $\text{MVEE}(\mathcal{S})$ satisfies

$$(1/d)\text{MVEE}(\mathcal{S}) \subseteq \text{conv}(\mathcal{S}) \subseteq \text{MVEE}(\mathcal{S}), \quad (2)$$

where $\text{conv}(\mathcal{S})$ denotes the convex hull of \mathcal{S} and the ellipsoid on the left-hand side is obtained by scaling the $\text{MVEE}(\mathcal{S})$ around its center by the factor $1/d$. Therefore, if \mathcal{S} is viewed as the set of vertices of a full-dimensional polytope $\mathcal{P} \subseteq \mathbb{R}^d$, then the $\text{MVEE}(\mathcal{S})$ yields a rounded approximation of \mathcal{P} .

Given $\epsilon > 0$, an ellipsoid $\mathcal{E}_{Q,c}$ is said to a $(1 + \epsilon)$ -approximation to the $\text{MVEE}(\mathcal{S})$ if

$$\mathcal{E}_{Q,c} \supseteq \mathcal{S}, \quad \text{vol } \mathcal{E}_{Q,c} \leq (1 + \epsilon) \text{vol } \text{MVEE}(\mathcal{S}). \quad (3)$$

Several algorithms have been developed for the MVEE problem. These algorithms can be categorized as first-order algorithms (Refs. 2, 10, 16–17), second-order interior-point algorithms (Refs. 18–19), and combination of the two (Ref. 17). For small dimensions d , the MVEE problem can be solved in $\mathcal{O}(d^{O(d)}n)$ operations using randomized (Refs. 3, 20–21) or deterministic (Ref. 4) algorithms. A fast implementation is also available in the CGAL library⁴ for solving the problem in two dimensions (Ref. 22). Khachiyan and Todd (Ref. 23) established a linear-time reduction of the MVEE problem to the problem of computing a maximum-volume inscribed ellipsoid (MVIE) in a polytope described by a finite number of inequalities. Therefore, the MVEE problem can be solved also using the algorithms developed for the MVIE problem (Refs. 23–27). Since the MVEE problem can be formulated as a maximum determinant problem, the more general algorithms of Vandenberghe et al. (Ref. 28) and Toh (Ref. 29) can be applied.

⁴See <http://www.cgal.org>.

In contrast to the previous results, we focus mainly on the instances of the MVEE problem with $|\mathcal{S}| = n \gg d$, which is satisfied by several application such as data mining and clustering. In particular, our goal is to compute a small subset $\mathcal{X} \subseteq \mathcal{S}$ such \mathcal{X} provides a good approximation of \mathcal{S} . For a point set \mathcal{S} , we say that $\mathcal{X} \subseteq \mathcal{S}$ is an ϵ -core set (or a core set) for \mathcal{S} (Refs. 30–32) if there exists an ellipsoid $\mathcal{E}_{Q,c} \subseteq \mathbb{R}^d$ such that $\mathcal{S} \subseteq \mathcal{E}_{Q,c}$ and $\mathcal{E}_{Q,c}$ is a $(1+\epsilon)$ -approximation to the MVEE(\mathcal{X}). It follows from this definition that a core set \mathcal{X} satisfies

$$\begin{aligned} \text{vol MVEE}(\mathcal{X}) &\leq \text{vol MVEE}(\mathcal{S}) \\ &\leq \text{vol } \mathcal{E}_{Q,c} \\ &\leq (1+\epsilon) \text{vol MVEE}(\mathcal{X}) \\ &\leq (1+\epsilon) \text{vol MVEE}(\mathcal{S}), \end{aligned}$$

which implies that $\mathcal{E}_{Q,c}$ is simultaneously a $(1+\epsilon)$ -approximation to the MVEE(\mathcal{X}) and MVEE(\mathcal{S}).

The identification of small core sets is an important step toward solving larger problems. Recently, core sets have received significant attention and small core set results have been established for several geometric optimization problems such as the minimum enclosing ball problem and related clustering problems (Refs. 30–34). Small core set results form a basis for developing practical algorithms for large-scale problems, since many geometric optimization problems can be solved efficiently for small input sets. In particular, the MVEE problem for an input set of m points in \mathbb{R}^d can be solved in $O(m^{3.5} \log(m/\epsilon))$ arithmetic operations (Ref. 17), which is the best known complexity result if d is not fixed.

In this paper, we propose a modification of the Khachiyan first-order algorithm (Ref. 17), which computes a $(1+\epsilon)$ -approximation to the MVEE(\mathcal{S}) in

$$\Phi(n, d, \epsilon) := O(nd^2[(1+\epsilon)^{(2/d+1)} - 1]^{-1} + \log d + \log \log n) \quad (4)$$

operations. Based on a simple initial volume approximation algorithm, our modification yields a complexity bound of

$$\Xi(n, d, \epsilon) := O(nd^2[(1+\epsilon)^{(2/d+1)} - 1]^{-1} + \log d) \quad (5)$$

arithmetic operations, which reduces (4) by $O(nd^2 \log \log n)$. In particular, our algorithm terminates in $O(nd^3/\epsilon)$ operations for $\epsilon \in (0, 1]$. As a byproduct, we establish the existence of an ϵ -core set $\mathcal{X} \subseteq \mathcal{S}$ such that

$$|\mathcal{X}| = O(d[(1+\epsilon)^{2/d+1} - 1]^{-1} + d \log d), \quad (6)$$

independent of n , the number of points in \mathcal{S} . In particular,

$$|\mathcal{X}| = O(d^2/\epsilon), \quad \text{for } \epsilon \in (0, 1].$$

We remark that any ellipsoid in \mathbb{R}^d is determined by at most $d(d+1)/2$ points, which implies that, in theory, there exists always a core set of size $O(d^2)$ for any $\epsilon \geq 0$. In comparison, our algorithm can compute efficiently a core set \mathcal{X} satisfying (6).

The paper is organized as follows. We define notation in the remainder of this section. In Section 2, we review formulations of the MVEE problem as an optimization problem. Section 3 is devoted to a deterministic volume-approximation algorithm that will be the basis for our algorithm. In Section 4, we review the Khachiyan first-order algorithm and its analysis and propose a new interpretation. We present our modification and establish a slightly improved complexity bound. As a byproduct, our algorithm returns a core set whose size is independent of n . Section 5 concludes the paper with future research directions.

1.1. Notation. Vectors will be denoted by lower-case Roman letters. For a vector u , u_i denotes the i th component. Inequalities on vectors will apply to each component. e will be reserved for the vector of ones in the appropriate dimension, which will be clear from the context. e_j is the j th unit vector. For a vector u , U will denote the diagonal matrix whose entries are given by the components of u . Upper-case Roman letters will be reserved for matrices. The identity matrix will be denoted by I . $\text{trace}(U)$ will denote the sum of the diagonal entries of U . For a finite set of vectors \mathcal{V} , $\text{span}(\mathcal{V})$ denotes the linear subspace spanned by \mathcal{V} . Functions and operators will be denoted by upper-case Greek letters. Except for n and d , scalars will be represented by lower-case Greek letters unless they represent the components of a vector or a sequence of scalars, vectors, or matrices. i, j, k will be reserved for indexing purposes. Upper-case script letters will be used for all other objects such as sets, polytopes, and ellipsoids.

2. Formulations

In this section, we discuss the formulations of the MVEE problem as an optimization problem. Throughout the rest of this paper, we make the following assumption, which guarantees that the minimum volume enclosing ellipsoid is full-dimensional:

$$(A1) \quad \text{The affine hull of } p^1, \dots, p^n \text{ is } \mathbb{R}^d.$$

The MVEE problem can be formulated as an optimization problem in several different ways (see e.g. Ref. 19). We consider two formulations in this section.

Given a set $\mathcal{S} \subseteq \mathbb{R}^d$ of n points p^1, \dots, p^n , we define a lifting of \mathcal{S} to \mathbb{R}^{d+1} via

$$\mathcal{S}' := \{\pm q^1, \dots, \pm q^n\}, \quad \text{where } q^i := [(p^i)^T, 1]^T, \quad i = 1, \dots, n. \quad (7)$$

From the results of Ref. 23 and Ref. 18, it follows that

$$\text{MVEE}(\mathcal{S}) = \text{MVEE}(\mathcal{S}') \cap \mathcal{H}, \quad (8)$$

where

$$\mathcal{H} := \{x \in \mathbb{R}^{d+1} : x_{d+1} = 1\}. \quad (9)$$

Since \mathcal{S}' is centrally symmetric, the $\text{MVEE}(\mathcal{S}')$ is centered at the origin. This observation gives rise to the following convex optimization problem to compute the $\text{MVEE}(\mathcal{S}')$, whose solution can be used to compute the $\text{MVEE}(\mathcal{S})$ via (8):

$$\begin{aligned} (\text{P}(\mathcal{S})) \quad & \min_M \quad -\log \det M, \\ & \text{s.t.} \quad (q^i)^T M q^i \leq 1, \quad i = 1, \dots, n, \\ & \quad M \in \mathbb{R}^{(d+1) \times (d+1)} \text{ is symmetric and positive definite,} \end{aligned}$$

where $M \in \mathbb{R}^{(d+1) \times (d+1)}$ is the decision variable. A positive-definite matrix $M^* \in \mathbb{R}^{(d+1) \times (d+1)}$ is optimal for $(\text{P}(\mathcal{S}))$ along with the Lagrange multipliers $z^* \in \mathbb{R}^n$ if and only if

$$-(M^*)^{-1} + \Pi(z^*) = 0, \quad (10a)$$

$$z_i^* (1 - (q^i)^T M^* q^i) = 0, \quad i = 1, \dots, n, \quad (10b)$$

$$(q^i)^T M^* q^i \leq 1, \quad i = 1, \dots, n, \quad (10c)$$

$$z^* \geq 0, \quad (10d)$$

where $\Pi: \mathbb{R}^n \rightarrow \mathbb{R}^{(d+1) \times (d+1)}$ is a linear operator given by

$$\Pi(z) := \sum_{i=1}^n z_i q^i (q^i)^T. \quad (11)$$

The Lagrangian dual of $(\text{P}(\mathcal{S}))$ is equivalent to

$$(\text{D}(\mathcal{S})) \quad \max_u \quad \log \det \Pi(u), \quad (12a)$$

$$\text{s.t.} \quad e^T u = 1, \quad (12b)$$

$$u \geq 0. \quad (12c)$$

where $u \in \mathbb{R}^n$ is the decision variable. Since $(D(S))$ is a concave maximization problem, $u^* \in \mathbb{R}^n$ is an optimal solution (along with the dual solutions $s^* \in \mathbb{R}^n$ and $\lambda^* \in \mathbb{R}$) if and only if the following optimality conditions are satisfied:

$$(q^i)^T \Pi(u^*)^{-1} q^i + s_i^* = \lambda^*, \quad i = 1, \dots, n, \quad (13a)$$

$$e^T u^* = 1, \quad (13b)$$

$$u_i^* s_i^* = 0, \quad i = 1, \dots, n, \quad (13c)$$

together with $u^* \geq 0$ and $s^* \geq 0$. Multiplying both sides of (13a) by u_i^* and summing up for $i = 1, \dots, n$ yields

$$\begin{aligned} \sum_{i=1}^n u_i^* (q^i)^T \Pi(u^*)^{-1} q^i &= \text{trace} \left\{ \Pi(u^*)^{-1} \left[\sum_{i=1}^n u_i^* q^i (q^i)^T \right] \right\} \\ &= \text{trace}(I) \\ &= d + 1, \end{aligned}$$

which implies

$$\lambda^* = d + 1,$$

by (13b) and (13c). Consequently,

$$M^* := [1/(d+1)] \Pi(u^*)^{-1} \quad (14)$$

is a feasible solution for $(P(S))$ and satisfies the optimality conditions (10) for $(P(S))$ together with

$$z^* := (d+1)u^*.$$

It follows from (8) and (14) that an optimal solution u^* for $(D(S))$ can be used to compute the MVEE(S) as follows:

$$\text{MVEE}(S) = \left\{ x \in \mathbb{R}^d : [1/(d+1)] [x^T, 1] \Pi(u^*)^{-1} \begin{bmatrix} x \\ 1 \end{bmatrix} \leq 1 \right\}. \quad (15)$$

Let $P \in \mathbb{R}^{d \times n}$ be the matrix whose i th column is given by p^i . By (11), we have

$$\begin{aligned} \Pi(u^*) &= \begin{bmatrix} P U^* P^T & P u^* \\ (P u^*)^T & 1 \end{bmatrix} \\ &= \begin{bmatrix} I & P u^* \\ 0 & 1 \end{bmatrix} \begin{bmatrix} P U^* P^T - P u^* (P u^*)^T & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} I & 0 \\ (P u^*)^T & 1 \end{bmatrix}. \end{aligned} \quad (16)$$

Inverting both sides in (16) yields

$$\Pi(u^*)^{-1} = \begin{bmatrix} I & 0 \\ -(Pu^*)^T & 1 \end{bmatrix} \begin{bmatrix} (PU^*P^T - Pu^*(Pu^*)^T)^{-1} & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} I - Pu^* \\ 0 & 1 \end{bmatrix}. \quad (17)$$

Substituting (17) in (15), we obtain

$$\text{MVEE}(S) = \mathcal{E}_{Q^*, c^*} := \{x \in \mathbb{R}^d : (x - c^*)^T Q^* (x - c^*) \leq 1\}, \quad (18)$$

where

$$Q^* := (1/d)(PU^*P^T - Pu^*(Pu^*)^T)^{-1}, \quad c^* := Pu^*. \quad (19)$$

This establishes the following result.

Lemma 2.1. Let $u^* \in \mathbb{R}^n$ be an optimal solution of (D(S)) and let $P \in \mathbb{R}^{d \times n}$ be the matrix whose i th column is given by p^i . Then, the $\text{MVEE}(S) = \mathcal{E}_{Q^*, c^*}$, where $Q^* \in \mathbb{R}^{d \times d}$ and $c^* \in \mathbb{R}^d$ are given by (19). Furthermore,

$$\log \text{vol MVEE}(S) = \log \eta + (d/2) \log d + (1/2) \log \det \Pi(u^*), \quad (20)$$

where η is the volume of the unit ball in \mathbb{R}^d .

Proof. We need only to prove (20). Note that

$$\text{vol MVEE}(S) = \eta \det(Q^*)^{-1/2},$$

where Q^* is defined as in (19). Therefore,

$$\begin{aligned} \log \text{vol MVEE}(S) &= \log \eta + (d/2) \log d \\ &\quad + (1/2) \log \det(PU^*P^T - Pu^*(Pu^*)^T). \end{aligned} \quad (21)$$

By (16),

$$\log \det \Pi(u^*) = \log \det(PU^*P^T - Pu^*(Pu^*)^T),$$

establishing (20). □

3. Initial Volume Approximation

Given $\mathcal{S} = \{p^1, \dots, p^n\} \subseteq \mathbb{R}^d$, we present a simple deterministic algorithm that identifies a subset $\mathcal{X}_0 \subseteq \mathcal{S}$ of size at most $2d$ such that $\text{vol MVEE}(\mathcal{X}_0)$ is a provable approximation to $\text{vol MVEE}(\mathcal{S})$.

Lemma 3.1. Algorithm 3.1 terminates in $O(nd^2)$ time with subset $\mathcal{X}_0 \subseteq \mathcal{S}$, with $|\mathcal{X}_0| \leq 2d$ such that

$$\text{vol MVEE}(\mathcal{S}) \leq d^{2d} \text{vol MVEE}(\mathcal{X}_0). \quad (22)$$

Proof. If $n \leq 2d$, then the result holds trivially. For $n > 2d$, the proof is based on the results of Ref. 35 and Ref. 36. At step k of Algorithm 3.1, Ψ is given by the span of k linearly independent vectors by Assumption A1. Hence, upon termination, $\Psi = \mathbb{R}^d$. It follows that $|\mathcal{X}_0| = 2d$. Note that each step requires $O(nd)$ operations, giving an overall running time of $O(nd^2)$ at the end of d steps. From the results of Ref. 35, it follows that

$$\text{vol conv}(\mathcal{S}) \leq d! \text{vol conv}(\mathcal{X}_0).$$

Combining this inequality with (2), we have

$$\begin{aligned} (1/d^d) \text{vol MVEE}(\mathcal{S}) &\leq \text{vol conv}(\mathcal{S}) \\ &\leq d! \text{vol conv}(\mathcal{X}_0) \\ &\leq d! \text{vol MVEE}(\mathcal{X}_0), \end{aligned}$$

which implies that

$$\text{vol MVEE}(\mathcal{S}) \leq d! d^d \text{vol MVEE}(\mathcal{X}_0) \leq d^{2d} \text{vol MVEE}(\mathcal{X}_0). \quad \square$$

Algorithm 3.1. Volume Approximation Algorithm.

- Step 0. Input the set of points $\mathcal{S} = \{p^1, \dots, p^n\} \subseteq \mathbb{R}^d$.
- Step 1. If $n \leq 2d$, then $\mathcal{X}_0 \leftarrow \mathcal{S}$. Return.
- Step 2. $\Psi \leftarrow \{0\}$, $\mathcal{X}_0 \rightarrow \emptyset$, $i \leftarrow 0$.
- Step 3. While $\mathbb{R}^d \setminus \Psi \neq \emptyset$, do Steps 4–8 below.
- Step 4. $i \leftarrow i + 1$.
- Step 5. Pick an arbitrary direction $b^i \in \mathbb{R}^d$ in the orthogonal complement of Ψ .
- Step 6. $\alpha \leftarrow \arg \max_{k=1, \dots, n} (b^i)^T p^k$, $\mathcal{X}_0 \leftarrow \mathcal{X}_0 \cup \{p^\alpha\}$.
- Step 7. $\beta \leftarrow \arg \min_{k=1, \dots, n} (b^i)^T p^k$, $\mathcal{X}_0 \leftarrow \mathcal{X}_0 \cup \{p^\beta\}$.
- Step 8. $\Psi \leftarrow \text{Span}(\Psi, \{p^\beta - p^\alpha\})$.

4. First-Order Algorithm

In this section, we present a modification of the Khachiyan first-order algorithm for approximating the minimum-volume enclosing ellipsoid of a given set $\mathcal{S} = \{p^1, \dots, p^n\} \subseteq \mathbb{R}^d$. Our modification leads to a slightly improved complexity bound. As a byproduct, our analysis establishes the existence of a core set $\mathcal{X} \subseteq \mathcal{S}$ whose size depends on only d and ϵ , but not on the number of points n .

4.1. Khachiyan Algorithm Revisited. The Khachiyan first-order algorithm in Ref. 17 can be interpreted in several different ways [e.g. barycentric coordinate descent (Ref. 17), conditional gradient method (Ref. 19)]. In this paper, we present our interpretation of this algorithm.

For a set of points $\mathcal{S} \subseteq \mathbb{R}^d$, consider the nonlinear optimization problem (D(\mathcal{S})). Given a feasible solution $u^i \in \mathbb{R}^n$, consider the following linearization of (D(\mathcal{S})) at u^i :

$$\begin{aligned} (\text{LP}_i) \quad & \max_{v \in \mathbb{R}^n} \sum_{k=1}^n v_k (q^k)^T \Pi(u^i)^{-1} q^k, \\ \text{s.t.} \quad & e^T v = 1, \quad v \geq 0. \end{aligned}$$

Since the feasible region of (LP_{*i*}) is the unit simplex in \mathbb{R}^n , the optimal solution v^* is the unit vector e_j , where

$$j := \arg \max_{k=1, \dots, n} (q^k)^T \Pi(u^i)^{-1} q^k. \quad (23)$$

Let

$$\kappa^i := \max_{k=1, \dots, n} (q^k)^T \Pi(u^i)^{-1} q^k. \quad (24)$$

The next iterate u^{i+1} is given by a convex combination of u^i and e_j , i.e.,

$$u^{i+1} := (1 - \beta^i) u^i + \beta^i e_j,$$

where β^i is the maximizer of the following one-dimensional optimization problem (see Ref. 17):

$$\begin{aligned} \beta^i &:= \arg \max_{\beta \in [0, 1]} \log \det \Pi((1 - \beta) u^i + \beta e_j) \\ &= [\kappa^i - (d + 1)] / [(d + 1)(\kappa^i - 1)]. \end{aligned} \quad (25)$$

The algorithm continues in an iterative manner starting with u^{i+1} . Consequently, the Khachiyan first-order method can be viewed as a sequential linear programming algorithm for the nonlinear optimization problem $D(S)$.

Upon termination, the algorithm returns an ellipsoid $\mathcal{E}_{Q,c}$ with the property that

$$S \subseteq \mathcal{E}_{Q,c}, \quad \text{vol } \mathcal{E}_{Q,c} \leq (1 + \epsilon) \text{ vol MVEE}(S), \quad (26)$$

where $\epsilon > 0$.

Algorithm 4.1 below outlines the Khachiyan algorithm.

4.2. Analysis of the Khachiyan Algorithm. Khachiyan proved the following complexity result.

Theorem 4.1. (See Ref. 17) Let $\epsilon > 0$. Algorithm 4.1 returns an ellipsoid $\mathcal{E}_{Q,c}$ that satisfies the conditions in (26) in $\Phi(n, d, \epsilon)$ operations, where Φ is defined by (4). In particular, if $\epsilon \in (0, 1)$, Algorithm 4.1 terminates after $o(nd^2(d/\epsilon + \log \log n))$ operations.

Algorithm 4.1. Khachiyan first-order algorithm.

- Step 0. Input the set of points $S = \{p^1, \dots, p^n\} \subseteq \mathbb{R}^d$, $\epsilon > 0$.
- Step 1. $i \leftarrow 0, u^0 \leftarrow (1/n)e$.
- Step 2. While not converged, execute Steps 3–5 below.
- Step 3. $j \leftarrow \arg \max_{k=1, \dots, n} (q^k)^T \Pi(u^i)^{-1} q^k$,
 $\kappa \leftarrow \max_{k=1, \dots, n} (q^k)^T \Pi(u^i)^{-1} q^k$.
- Step 4. $\beta \leftarrow [\kappa - (d+1)] / [(d+1)(\kappa - 1)]$.
- step 5. $u^{i+1} \leftarrow (1 - \beta)u^i + \beta e_j, i \leftarrow i + 1$.

In this section, we present our interpretation of the analysis of Algorithm 4.1. Let $S' \subseteq \mathbb{R}^{d+1}$ denote the lifting of the point set $S \subseteq \mathbb{R}^d$ given by (7). It follows from (8) that the MVEE(S) can be recovered from the MVEE(S'). Furthermore, if the ellipsoid $\tilde{\mathcal{E}} \subseteq \mathbb{R}^{d+1}$ is a $(1+\epsilon)$ -approximation of the MVEE(S'), then

$$\mathcal{E} := \tilde{\mathcal{E}} \cap \mathcal{H} \subseteq \mathbb{R}^d$$

is a $(1+\epsilon)$ -approximation of the MVEE(S), where \mathcal{H} is given by (9) (see Refs. 18, 23). Therefore, we analyze Algorithm 4.1 for $S' \subseteq \mathbb{R}^{d+1}$.

At iteration i , we define a trial ellipsoid [cf. (14)]

$$\tilde{\mathcal{E}}^i := \tilde{\mathcal{E}}_{M^i, 0} \subseteq \mathbb{R}^{d+1},$$

where

$$M^i := [1/(d+1)] \Pi(u^i)^{-1}, \quad i = 0, 1, 2, \dots \quad (27)$$

Note that one can define a corresponding ellipsoid $\mathcal{E}^i := \mathcal{E}_{Q^i c^i} \subseteq \mathbb{R}^d$ via (19),

$$Q^i := (1/d)(PU^i P^T - (Pu^i)(Pu^i)^T)^{-1}, \quad c^i := Pu^i, \quad i = 0, 1, 2, \dots \quad (28)$$

Furthermore, by (27),

$$\begin{aligned} \text{vol } \tilde{\mathcal{E}}^i &= \eta' \det(M^i)^{-1/2} \\ &= \eta' (d+1)^{(d+1)/2} \det \Pi(u^i)^{1/2}, \end{aligned}$$

where η' is the volume of the unit ball in \mathbb{R}^{d+1} . Therefore,

$$\begin{aligned} \log \text{vol } \tilde{\mathcal{E}}^i &= \log \eta' + [(d+1)/2] \log(d+1) \\ &\quad + (1/2) \log \det \Pi(u^i), \quad i = 0, 1, 2, \dots \end{aligned} \quad (29)$$

Similarly to (20), we have

$$\begin{aligned} \log \text{vol } \mathcal{E}^i &= \log \eta + (d/2) \log d \\ &\quad + (1/2) \log \det \Pi(u^i), \quad i = 0, 1, 2, \dots, \end{aligned} \quad (30)$$

which together with (29) implies that $\log \text{vol } \tilde{\mathcal{E}}^i$ and $\log \text{vol } \mathcal{E}^i$ differ by a constant that depends on only d .

Let u^* denote the optimal solution of $(D(S))$. Since u^i is feasible solution of $(D(S))$, it follows from (29) and (14) that

$$\text{vol } \tilde{\mathcal{E}}^i \leq \text{vol MVEE}(S'), \quad i = 0, 1, 2, \dots \quad (31)$$

We define

$$\epsilon_i := \min\{v \geq 0 : (q^k)^T M^i (q^k) \leq 1 + v, \quad k = 1, \dots, n\}, \quad i = 0, 1, 2, \dots, \quad (32)$$

so that

$$S' \subseteq \sqrt{1 + \epsilon_i} \tilde{\mathcal{E}}^i.$$

ϵ_i can be viewed as a quality measure of iterate i . Combining (31) and (32), we obtain

$$\begin{aligned} \text{vol } \tilde{\mathcal{E}}^i &\leq \text{MVEE}(S') \\ &\leq (1 + \epsilon_i)^{(d+1)/2} \text{vol } \tilde{\mathcal{E}}^i, \quad i = 0, 1, 2, \dots \end{aligned} \quad (33)$$

Taking logarithms in (33), it follows from (29) that

$$v_i \leq v^* \leq (d+1) \log(1 + \epsilon_i) + v_i, \quad i = 0, 1, 2, \dots, \quad (34)$$

where v_i denotes the objective function value corresponding to the feasible solution u^i of $(D(\mathcal{S}))$, i.e.,

$$v_i := \log \det \Pi(u^i), \quad i = 0, 1, 2, \dots, \quad (35)$$

and v^* denotes the optimal value of $(D(\mathcal{S}))$.

By (32) and (27), we have

$$\begin{aligned} \kappa^i &:= \max_{k=1, \dots, n} (q^k)^T \Pi(u^i)^{-1} q^k \\ &= (d+1)(1 + \epsilon_i), \quad i = 0, 1, 2, \dots, \end{aligned} \quad (36)$$

so that

$$\beta^i := [\kappa^i - (d+1)] / [(d+1)(\kappa^i - 1)] = \epsilon_i / (\kappa^i - 1), \quad i = 0, 1, 2, \dots \quad (37)$$

The next iterate u^{i+1} is defined as

$$u^{i+1} := (1 - \beta^i)u^i + \beta^i e_j, \quad (38)$$

where j and β^i are given by (23) and (25), respectively. Since $\Pi(u)$ is linear, we obtain

$$\begin{aligned} \Pi(u^{i+1}) &= (1 - \beta^i)\Pi(u^i) + \beta^i \Pi(e_j) \\ &= \Pi(u^i)[(1 - \beta^i)I + \beta^i \Pi(u^i)^{-1} \Pi(e_j)]. \end{aligned} \quad (39)$$

Arguing similarly to Lemma 3 of Ref. 17, we have

$$\begin{aligned} \log \det \Pi(u^{i+1}) &= \log \det \Pi(u^i) + d \log(1 - \beta^i) + \log(1 + \epsilon_i) \\ &= \log \det \Pi(u^i) - d \log[1 + \epsilon_i / d(1 + \epsilon_i)] + \log(1 + \epsilon_i) \\ &\geq \log \det \Pi(u^i) - \epsilon_i / (1 + \epsilon_i) + \log(1 + \epsilon_i), \quad i = 0, 1, 2, \dots, \\ &\geq \log \det \Pi(u^i) + \begin{cases} \log 2 - 1/2 > 0, & \text{if } \epsilon_i \geq 1, \\ (1/8)\epsilon_i^2, & \text{if } \epsilon_i < 1 \end{cases} \end{aligned} \quad (40)$$

which implies that the objective function value strictly increases at each iteration.

Note that

$$\begin{aligned} \kappa^0 &= \max_{k=1, \dots, n} (q^k)^T \Pi(u^0)^{-1} q^k \\ &\leq \sum_{k=1}^n (q^k)^T \Pi(u^0)^{-1} q^k \end{aligned}$$

$$\begin{aligned}
&= n \operatorname{trace} \Pi(e)^{-1} \Pi(e) \\
&= n(d+1).
\end{aligned}$$

By (36), it follows that

$$\epsilon_0 \leq n - 1. \quad (41)$$

The following inequalities follow from (34), (40), and (41):

$$\nu_0 > -\infty, \quad (42a)$$

$$\begin{aligned}
\delta_i &:= \nu^* - \nu_i \\
&\leq (d+1) \log(1 + \epsilon_i), \quad i = 0, 1, \dots,
\end{aligned} \quad (42b)$$

$$\begin{aligned}
\Pi &:= \nu_{i+1} - \nu_i \\
&\geq \log(1 + \epsilon_i) - \epsilon_i / (1 + \epsilon_i), \quad i = 0, 1, \dots,
\end{aligned} \quad (42c)$$

$$\begin{aligned}
\delta_0 &= \nu^* - \nu_0 \\
&\leq (d+1) \log n.
\end{aligned} \quad (42d)$$

The Khachiyan analysis of Algorithm 4.1 (see Lemma 4 in Ref. 17) consists of two stages. In the first stage, an upper bound is derived on the smallest index k such that $\epsilon_k \leq 1$. Using (42b) and (42c), Khachiyan establishes that

$$k = O(d \log \delta_0), \quad (43)$$

which implies that, by (42d),

$$k = O(d(\log d + \log \log n)).$$

The second stage of the Khachiyan analysis consists of bounding the number of iterations to halve ϵ_i assuming $\epsilon \leq 1$. Khachiyan shows that it takes $O(d/\mu)$ iterations to obtain $\epsilon_i \leq \mu$ for any $\mu \in (0, 1)$. It follows from (33) that Algorithm 4.1 needs to run until

$$\epsilon \leq (1 + \epsilon)^{2/d+1} - 1 \quad (44)$$

in order to obtain a $(1 + \epsilon)$ -approximation to the MVEE(\mathcal{S}).

Combining the two parts together with the fact that each iteration can be performed in $O(nd)$ operations via updating $\Pi(u^i)^{-1}$ using (39) yields the complexity result of Theorem 4.1. If $\epsilon \in (0, 1)$, then

$$(1 + \epsilon)^{2/(d+1)} - 1 = O(\epsilon/d),$$

proving the second part of Theorem 4.1.

4.3. Different Interpretation of the Khachiyan Algorithm. Our presentation of the analysis of the Khachiyan algorithm gives rise to another interpretation. Consider the trial ellipsoid $\mathcal{E}^i \subseteq \mathbb{R}^d$ corresponding to u^i defined by (28). By (17),

$$(q^k)^T \Pi(u^i)^{-1} q^k = d(p^k - c^i)^T Q^i (p^k - c^i) + 1, \quad k = 1, \dots, n. \quad (45)$$

At each iteration, it follows from (36) that the algorithm computes the farthest point p^j from the current trial ellipsoid \mathcal{E}^i using its ellipsoidal norm. By (38) and (28), the center c^{i+1} of the next trial ellipsoid $\mathcal{E}^{i+1} := \mathcal{E}_{Q^{i+1}, c^{i+1}}$ is shifted toward p^j , i.e.,

$$c^{i+1} = (1 - \beta^i) c^i + \beta^i p^j. \quad (46)$$

Similarly, by (28),

$$\begin{aligned} (Q^i)^{-1} &= d(PU^i P^T - (Pu^i)(Pu^i)^T) \\ &= d \sum_{k=1}^n u_k (p^k - c^i)(p^k - c^i)^T, \end{aligned}$$

where we used

$$\sum_{k=1}^n u_k = 1 \quad \text{and} \quad Pu^i = c^i.$$

By (38), it follows that

$$(Q^{i+1})^{-1} = (1 - \beta^i)(Q^i)^{-1} + d\beta(p^j - c^i)(p^j - c^i)^T, \quad (47)$$

which implies that the next trial ellipsoid is obtained by ‘expanding’ the current trial ellipsoid toward p^j . In particular, if $p^j - c^i$ coincides with one of the axes of \mathcal{E}^i (i.e., one of the eigenvectors of Q^i), then \mathcal{E}^{i+1} is simply obtained by expanding \mathcal{E}^i along that axis and shrinking it along the remaining axes.

Therefore, the Khachiyan algorithm generates implicitly a sequence of ellipsoids with the property that the next ellipsoid in the sequence is given by shifting and expanding the current ellipsoid towards the farthest outlier.

4.4. Modification. In this subsection, we present a modification of the Khachiyan first-order algorithm described in Section 4.1. Our algorithm leads to a slightly improved complexity bound.

Algorithm 4.2. It outputs a $(1 + \epsilon)$ -approximation of $\text{MVEE}(\mathcal{S})$

- Step 0. Input the set of points $\mathcal{S} = \{p^1, \dots, p^n\} \subseteq \mathbb{R}^d$, $\epsilon \in (0, 1)$.
 Step 1. Run Algorithm 3.1 on \mathcal{S} to get the output \mathcal{X}_0 .
 Step 2. Let $u^0 \in \mathbb{R}^n$ be such that $u_j^0 = 1/|\mathcal{X}_0|$ for $p^j \in \mathcal{X}_0$ and $u_j^0 = 0$, otherwise.
 Step 3. Run Algorithm 4.1 on \mathcal{S} starting with u^0 .

The following theorem gives a complexity bound for Algorithm 4.2.

Theorem 4.2. Let $\epsilon > 0$. Algorithm 4.2 returns a $(1 + \epsilon)$ -approximation of the $\text{MVEE}(\mathcal{S})$ in $\Xi(n, d, \epsilon)$ operations, where Ξ is defined by (5). In particular, if $\epsilon \in (0, 1)$, Algorithm 4.2 terminates after $O(nd^3/\epsilon)$ operations.

Proof. By Lemma 3.1, Algorithm 3.1 returns $\mathcal{X} \subseteq \mathcal{S}$ of size at most $2d$ in $O(nd^2)$ operations. Let $u_{\mathcal{X}_0} \in \mathbb{R}^{|\mathcal{X}_0|}$ denote the restriction of u^0 to its positive components. Since $u_{\mathcal{X}_0}$ coincides with the initial iterate in Algorithm 3.1 applied to $(D(\mathcal{X}_0))$, it follows from (42d) that

$$\log \det \Pi(u_*) - \log \det \Pi(u^0) = O(d \log d), \quad (48)$$

where $u_* \in \mathbb{R}^n$ denotes the vector whose restriction to its components in \mathcal{X}_0 yields the optimal of solution $(D(\mathcal{X}_0))$.

By Lemma 3.1,

$$\text{vol MVEE}(\mathcal{S}) \leq d^{2d} \text{vol MVEE}(\mathcal{X}_0).$$

Taking logarithms on both sides, it follows from (30) that

$$\log \det \Pi(u^*) - \log \det \Pi(u_*) = O(d \log d), \quad (49)$$

where u^* denotes the optimal solution of $(D(\mathcal{S}))$. By (48) and (49), we obtain

$$\log \det \Pi(u^*) - \log \det \Pi(u^0) = O(d \log d).$$

Since u^0 is used as an initial iterate in Algorithm 4.1, it follows from (42d) and (43) that Algorithm 4.2 requires $O(d \log d)$ iterations to obtain an iterate u^i with $\epsilon_i \leq 1$. Combining this result with the second part of the analysis of Algorithm 4.1, we obtain the desired complexity result. \square

4.5. Core Set Result. In this subsection, we establish that, upon termination, our algorithm produces a core set $\mathcal{X} \subseteq \mathcal{S}$ whose size depends on only d and ϵ , but not on n .

Theorem 4.3. Let $\epsilon > 0$. For a given $\mathcal{S} = \{p^1, \dots, p^n\} \subseteq \mathbb{R}^d$ of n points, let u^f denote the final iterate returned by Algorithm 4.2 applied to \mathcal{S} . Let $\mathcal{X} := \{p^k \in \mathcal{S} : u_k^f > 0, k = 1, \dots, n\}$. Then, \mathcal{X} is an ϵ -core set of \mathcal{S} . Furthermore,

$$|\mathcal{X}| = O(d[(1+\epsilon)^{2/d+1} - 1]^{-1} + d \log d). \quad (50)$$

In particular, if $\epsilon \in (0, 1)$, then

$$|\mathcal{X}| = O(d^2/\epsilon).$$

Proof. We first prove (50). Note that u^0 in Algorithm 4.2 has at most $2d$ positive components and that, at each iteration, at most one component becomes positive. Therefore,

$$\begin{aligned} |\mathcal{X}| &\leq 2d + O(d \log d + d[(1+\epsilon)^{2/d+1} - 1]^{-1}) \\ &= O(d[(1+\epsilon)^{2/d+1} - 1]^{-1} + d \log d). \end{aligned}$$

Let $\tilde{\mathcal{E}}^f \subseteq \mathbb{R}^{d+1}$ denote the trial ellipsoid corresponding to u^f defined via (27) and let

$$\tilde{\mathcal{E}} := (1+\epsilon)^{1/d+1} \tilde{\mathcal{E}}^f.$$

By (44),

$$\text{conv}(\mathcal{X}') \subseteq \text{conv}(\mathcal{S}') \subseteq \tilde{\mathcal{E}}, \quad (51)$$

where \mathcal{X}' and \mathcal{S}' denote the lifting of \mathcal{X} and \mathcal{S} to \mathbb{R}^{d+1} , respectively. By (33), we have

$$\begin{aligned} \text{vol } \tilde{\mathcal{E}}^f &\leq \text{vol MVEE}(\mathcal{S}') \\ &\leq (1+\epsilon) \text{vol } \tilde{\mathcal{E}}^f \\ &= \text{vol } \tilde{\mathcal{E}}, \end{aligned} \quad (52)$$

which implies that

$$\text{vol } \tilde{\mathcal{E}} \leq (1+\epsilon) \text{vol MVEE}(\mathcal{S}').$$

Let $u_{\mathcal{X}}^f \in \mathbb{R}^{|\mathcal{X}|}$ be the restriction of u^f to its positive components. Note that $u_{\mathcal{X}}^f$ is a feasible solution of $(D(\mathcal{X}))$. Furthermore, the trial ellipsoid corresponding to $u_{\mathcal{X}}^f$ coincides with $\tilde{\mathcal{E}}^f$ by (27). Therefore, arguing similarly to (31), we obtain

$$\begin{aligned} [1/(1+\epsilon)] \text{vol } \tilde{\mathcal{E}} &= \text{vol } \tilde{\mathcal{E}}^f \\ &\leq \text{vol MVEE}(\mathcal{X}'), \end{aligned} \quad (53)$$

which, together with (52), implies that

$$\begin{aligned} \text{vol MVEE}(\mathcal{X}') &\leq \text{vol MVEE}(S') \\ &\leq \text{vol } \tilde{\mathcal{E}} \\ &\leq (1+\epsilon) \text{vol MVEE}(\mathcal{X}') \\ &\leq (1+\epsilon) \text{vol MVEE}(S'). \end{aligned}$$

Since lifting preserves the approximation factor, it follows from (51)–(53) that the ellipsoid $\mathcal{E} := \tilde{\mathcal{E}} \cap \mathcal{H}$, where \mathcal{H} is defined by (9), is simultaneously a $(1+\epsilon)$ -approximation to $\text{MVEE}(\mathcal{X})$ and to $\text{MVEE}(S)$. Therefore, \mathcal{X} is an ϵ -core set of S . \square

Remark 4.1. The size of the core set \mathcal{X} in Theorem 4.3 depends on only d and ϵ and is independent of n . In several applications with $n \gg d$, our algorithm finds a $(1+\epsilon)$ -approximation in linear time in n and returns a core set whose size is independent of n . The identification of such a small set may play an important role in applications such as data classification.

Remark 4.2. The proof of Theorem 4.3 can be applied to the Khachiyan algorithm (i.e., Algorithm 4.1) as well and a core set can similarly be defined upon termination. However, Algorithm 4.1 uses an initial iterate all of whose components are positive. Therefore, for instances with $n \gg d$, Algorithm 4.1 will return S itself as a trivial core set. The reduction in the size of the core set is a consequence of using Algorithm 3.1 to obtain an initial iterate with a provably better lower bound on the optimal value of $(D(S))$.

Remark 4.3. Algorithm 4.2 does not lead to an improvement of the currently best-known complexity result of Khachiyan (Ref. 17) for the minimum-volume enclosing ellipsoid problem. The complexity results of the algorithms preceding the Khachiyan work (see Refs. 37, 18, 23) depend on $\log(R/r)$, where r and R denote the radii of two balls inscribed in

and circumscribing the convex hull of the given point set, respectively. In particular, Nesterov and Nemirovskii (Ref. 18) develop an interior-point algorithm that computes a $(1 + \epsilon)$ -approximation to the minimum-volume enclosing ellipsoid of a set of n points in \mathbb{R}^d in $O(n^{3.5} \log(Rn/r\epsilon))$ operations. The Khachiyan algorithm calls Algorithm 4.1 with $\epsilon = 1$, whose solution is used to obtain two balls with $R/r \leq 2d$, in $O(nd^2(\log d + \log \log n))$ operations and then uses the approximate solution as a warm-start in the interior-point algorithm, thereby reducing the overall complexity to $O(n^{3.5} \log(n/\epsilon))$ operations. The use of Algorithm 4.2 instead of Algorithm 4.1 in the Khachiyan algorithm would reduce only the complexity of the first stage to $O(nd^2 \log d)$ without having any effect on the complexity of the second stage, which determines the overall complexity.

5. Conclusions and Future Work

In this paper, we propose and analyze a first-order algorithm to compute an approximate minimum-volume enclosing ellipsoid of a given set of n points in \mathbb{R}^d . We establish that our algorithm returns a core set whose size depends on only d and ϵ . Especially for instances of the MVEE problem with $n \gg d$, our algorithm is capable of efficiently computing a small subset which provides a good representation of the input point set.

This paper is an addition to the recent thread of works on core sets for several geometric optimization problems (Refs. 30–34) and for the first time introduces the notion of core sets for minimum-volume enclosing ellipsoids.

Since most applications of the MVEE problem have relatively small dimension d and since ϵ is usually fixed, our algorithm has a complexity bound with the desirable property that its dependence on the number of points n is linear.

On the other hand, it is well-known that first-order algorithms suffer from slow convergence in practice especially for smaller values of ϵ . Several interior-point methods developed for the MVEE problem perform well in practice and can achieve higher accuracy in reasonable time (see e.g. Refs. 19, 23, 27). For instances of the MVEE problem with $n \gg d$, Sun and Freund (Ref. 19) propose and implement a practical column generation approach using an interior-point algorithm to solve each subproblem. Motivated by the core set result established in this paper and the encouraging computational results based on a core set result for the minimum enclosing ball problem (Ref. 32), we intend to work on a column generation algorithm for the minimum-volume enclosing ellipsoid problem with an emphasis on obtaining an upper bound on the number of columns

generated to obtain a desired accuracy. In particular, one of the algorithms in Ref. 32 uses a hybrid approach based on a first-order method and a column generation algorithm. Currently, we are experimenting with a similar idea for the minimum-volume enclosing ellipsoid problem.

There are several interesting problems associated with core sets. For instance, does there exist an input set of points that provides a lower bound on the size of core sets? Can one establish similar core set results for other geometric optimization problems? Does there exist a unifying framework for core sets in general? We intend to pursue these research problems in the near future.

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