Minimum Volume Enclosing Ellipsoids and Core Sets

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May 3, 2004

Abstract

Abstract. We study the problem of computing a $(1+\epsilon)$-approximation to the minimum volume enclosing ellipsoid of a given point set $\mathcal{S} = \{p^1, p^2, \ldots, p^n\} \subseteq \mathbb{R}^d$. Based on a simple, initial volume approximation method, we propose a modification of Khachiyan's 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 $\mathcal{X} \subseteq \mathcal{S}$ with the property that the minimum volume enclosing ellipsoid of $\mathcal{X}$ provides a good approximation to that of $\mathcal{S}$. Furthermore, the size of $\mathcal{X}$ depends only on 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 $\epsilon \in (0,1)$.

Keywords: Löwner ellipsoid, core sets, approximation algorithms.

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1 Introduction

We study the problem of computing the minimum volume enclosing ellipsoid (MVEE) of a given point set $\mathcal{S} = \{p^1, \ldots, p^n\} \subseteq \mathbb{R}^d$, denoted by MVEE($\mathcal{S}$), also known as the Löwner ellipsoid for $\mathcal{S}$. 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 such as 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

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

The volume of an ellipsoid $\mathcal{E}_{Q,c}$, denoted by vol $\mathcal{E}_{Q,c}$, is given by vol $\mathcal{E}_{Q,c} = \eta \det Q^{-\frac{1}{2}}$, where η is the volume of the unit ball in $\mathbb{R}^d$ (Ref. 6).

F. John in Ref. 15 proved that MVEE($\mathcal{S}$) satisfies

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

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

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

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

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 a combination of the two (Ref. 17). For small dimensions d, the MVEE problem can be solved in $O(d^{O(d)}n)$ operations using randomized (Refs. 3,20–21) or deterministic (Ref. 4) algorithms. A fast implementation is also available in the CGAL library[1] for solving the problem in two dimensions (Ref. 22). Khachiyan and Todd in 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 also be solved using the algorithms developed for the MVIE problem (Refs. 23–27). Since the MVEE problem can be formulated as a maximum determinant problem, more general algorithms of Vandenberghe et. al. in Ref. 28 and Toh in Ref. 29 can be applied.

In contrast to the previous results, we mainly focus on the instances of the MVEE problem with $|\mathcal{S}| = n \gg d$, which is satisfied by several applications such as data mining and clustering. In particular, our goal is to compute a small subset $\mathcal{X} \subseteq \mathcal{S}$ such that $\mathcal{X}$ 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 MVEE($\mathcal{X}$). It follows from this definition that a core

[1]http://www.cgal.org

set $\mathcal{X}$ satisfies

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

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

The identification of small core sets is an important step towards 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 (Ref. 32) and related clustering problems (Refs. 31,33–35). 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 Khachiyan's first-order algorithm (Ref. 17), which computes a $(1+\epsilon)$-approximation to MVEE($\mathcal{S}$) in

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

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

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

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

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

independent of n, the number of points in $\mathcal{S}$. In particular, $|\mathcal{X}| = O(d^2/\epsilon)$ 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 always exists a core set of size $O(d^2)$ for any $\epsilon \geq 0$. In comparison, our algorithm can efficiently compute 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 Khachiyan's 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 ith 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 jth unit vector. For a vector u, U will denote the diagonal matrix whose entries are given by components of u. Upper-case Roman letters will be reserved for matrices. The identity matrix will be denoted by I. trace(U) will denote the sum of the diagonal entries of U. For a finite set of vectors $\mathcal{V}$, span($\mathcal{V}$) denotes the linear subspace spanned by $\mathcal{V}$. Functions and operators will be denoted by upper-case Greek letters. Scalars except for n and d will be represented by lower-case Greek letters unless they represent components of a vector or a sequence of scalars, vectors or matrices. i, j, and 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 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.

Assumption 2.1 *The affine hull of* $p^1, \ldots, p^n$ *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 $p^1, \ldots, p^n$, we define a "lifting" of $\mathcal{S}$ to $\mathbb{R}^{d+1}$ via

$$\mathcal{S}' := \{\pm q^1, \ldots, \pm q^n\}, \quad \text{where} \quad q^i := \begin{bmatrix} p^i \\ 1 \end{bmatrix}, \quad i = 1, \ldots, n. \tag{7}$$

It follows from the results of Ref. 23 and Ref. 18 that

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

where

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

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

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

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 $(\mathbf{P}(\mathcal{S}))$ along with Lagrange multipliers $z^* \in \mathbb{R}^n$ if and only if

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

$$z_i^* \left(1 - (q^i)^T M^* \; q^i\right) \;=\; 0, \quad i = 1, \ldots, n, \tag{10b}$$

$$(q^i)^T M^* \; q^i \;\leq\; 1, \quad i = 1, \ldots, n, \tag{10c}$$

$$z^* \;\geq\; 0, \tag{10d}$$

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

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

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

$$\begin{array}{lll} (\mathbf{D}(\mathcal{S})) & \max_u & \log\det \Pi(u) \\ & \text{s.t.} & e^T u = 1, \\ & & u \geq 0, \end{array}$$

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

$$
\begin{aligned}
(q^i)^T \Pi(u^*)^{-1} q^i + s_i^* &= \lambda^*, \quad i = 1, \ldots, n, && \text{(13a)} \\
e^T u^* &= 1, && \text{(13b)} \\
u_i^* s_i^* &= 0, \quad i = 1, \ldots, n, && \text{(13c)}
\end{aligned}
$$

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

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

which implies $\lambda^* = d + 1$ by (13b) and (13c). Consequently,

$$M^* := \frac{1}{d+1} \Pi(u^*)^{-1} \tag{14}$$

is a feasible solution for $(\mathbf{P}(\mathcal{S}))$ and satisfies the optimality conditions (10) for $(\mathbf{P}(\mathcal{S}))$ together with $z^* := (d+1)u^*$.

It follows from (8) and (14) that an optimal solution u^* for $(\mathbf{D}(\mathcal{S}))$ can be used to compute $\mathrm{MVEE}(\mathcal{S})$ as follows:

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

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

$$\Pi(u^*) = \begin{bmatrix} PU^*P^T & Pu^* \\ (Pu^*)^T & 1 \end{bmatrix} = \begin{bmatrix} I & Pu^* \\ 0 & 1 \end{bmatrix} \begin{bmatrix} PU^*P^T - Pu^*(Pu^*)^T & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} I & 0 \\ (Pu^*)^T & 1 \end{bmatrix}. \tag{16}$$

Inverting both sides in (16) yields

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

Substituting (17) in (15), we obtain

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

where

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

This establishes the following result.

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

$$\log vol\ MVEE(\mathcal{S}) = \log \eta + \frac{d}{2} \log d + \frac{1}{2} \log \det \Pi(u^*), \tag{20}$$

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

Proof. We only need to prove (20). Note that vol MVEE$(\mathcal{S}) = \eta \det(Q^*)^{-\frac{1}{2}}$, where Q^* is defined as in (19). Therefore,

$$\log \text{vol MVEE}(\mathcal{S}) = \log \eta + \frac{d}{2} \log d + \frac{1}{2} \log \det \left(PU^*P^T - Pu^*(Pu^*)^T\right). \tag{21}$$

By (16), $\log \det \Pi(u^*) = \log \det(PU^*P^T - Pu^*(Pu^*)^T)$, establishing (20). $\square$

3 Initial Volume Approximation

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

Algorithm 1 Volume approximation algorithm

Require: Input set of points $\mathcal{S} = \{p^1, \ldots, p^n\} \subseteq \mathbb{R}^d$

If $n \leq 2d$, then $\mathcal{X}_0 \leftarrow \mathcal{S}$. Return.

$\Psi \leftarrow \{0\}$, $\mathcal{X}_0 \leftarrow \emptyset$, $i \leftarrow 0$.

While $\mathbb{R}^d \setminus \Psi \neq \emptyset$ do

loop

  $i \leftarrow i + 1$. Pick an arbitrary direction $b^i \in \mathbb{R}^d$ in the orthogonal complement of Ψ.

  $\alpha \leftarrow \arg\max_{k=1,\ldots,n} (b^i)^T p^k$, $\mathcal{X}_0 \leftarrow \mathcal{X}_0 \cup \{p^\alpha\}$.

  $\beta \leftarrow \arg\min_{k=1,\ldots,n} (b^i)^T p^k$, $\mathcal{X}_0 \leftarrow \mathcal{X}_0 \cup \{p^\beta\}$.

  $\Psi \leftarrow \text{span}(\Psi, \{p^\beta - p^\alpha\})$.

end loop

Lemma 3.1 *Algorithm 1 terminates in $O(nd^2)$ time with a subset $\mathcal{X}_0 \subseteq \mathcal{S}$ with $|\mathcal{X}_0| \leq 2d$ such that*

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

Proof. If $n \leq 2d$, then the result trivially holds. For $n > 2d$, the proof is based on the results of Ref. 36 and Ref. 37. At step k of Algorithm 1, Ψ is given by the span of k

linearly independent vectors by Assumption 2.1. 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. It follows from the results of Ref. 36 that vol conv$(\mathcal{S}) \leq d!$ vol conv$(\mathcal{X}_0)$. Combining this inequality with (2), we have

$$\frac{1}{d^d} \text{ vol MVEE}(\mathcal{S}) \leq \text{vol conv}(\mathcal{S}) \leq d! \text{ vol conv}(\mathcal{X}_0) \leq d! \text{ vol MVEE}(\mathcal{X}_0),$$

which implies that vol MVEE$(\mathcal{S}) \leq d! d^d$vol MVEE$(\mathcal{X}_0) \leq d^{2d}$ MVEE$(\mathcal{X}_0)$.

$\square$

4 A First-Order Algorithm

In this section, we present a modification of Khachiyan's first-order algorithm for approximating the minimum volume enclosing ellipsoid of a given set $\mathcal{S} = \{p^1, \ldots, p^n\} \subseteq \mathbb{R}^d$. 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 only on d and ϵ, but not on n, the number of points.

4.1 Khachiyan's Algorithm Revisited

Khachiyan's 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 ($\mathbf{D}(\mathcal{S})$). Given a feasible solution $u^i \in \mathbb{R}^n$, consider the following linearization of ($\mathbf{D}(\mathcal{S})$) at u^i:

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

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

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

Let

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

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):

$$\beta^i := \arg \max_{\beta \in [0,1]} \log \det \Pi((1 - \beta) u^i + \beta e_j) = \frac{\kappa^i - (d+1)}{(d+1)(\kappa^i - 1)}. \tag{25}$$

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

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

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

where $\epsilon > 0$.

Below, we outline Khachiyan's algorithm.

Algorithm 2 Khachiyan's first-order algorithm

Require: Input set of points $\mathcal{S} = \{p^1, \ldots, p^n\} \subseteq \mathbb{R}^d, \epsilon > 0$

$i \leftarrow 0$, $u^0 \leftarrow (1/n)e$

While not converged

loop

  $j \leftarrow \arg\max_{k=1,\ldots,n} (q^k)^T \Pi(u^i)^{-1} q^k$, $\kappa \leftarrow \max_{k=1,\ldots,n} (q^k)^T \Pi(u^i)^{-1} q^k$.

  $\beta \leftarrow \frac{\kappa-(d+1)}{(d+1)(\kappa-1)}$

  $u^{i+1} \leftarrow (1-\beta)u^i + \beta e_j$, $i \leftarrow i+1$.

end loop

4.1.1 Analysis of Khachiyan's Algorithm

Khachiyan proved the following complexity result.

Theorem 4.1 (Khachiyan (1993)) *Let $\epsilon > 0$. Algorithm 2 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 2 terminates after $O(nd^2(d/\epsilon + \log\log n))$ operations.*

In this section, we present our interpretation of the analysis of Algorithm 2. Let $\mathcal{S}' \subseteq \mathbb{R}^{d+1}$ denote the lifting of the point set $\mathcal{S} \subseteq \mathbb{R}^d$ given by (7). It follows from (8) that MVEE($\mathcal{S}$) can be recovered from MVEE($\mathcal{S}'$). Furthermore, if the ellipsoid $\tilde{\mathcal{E}} \subseteq \mathbb{R}^{d+1}$ is a $(1+\epsilon)$-approximation of MVEE($\mathcal{S}'$), then $\mathcal{E} := \tilde{\mathcal{E}} \cap \mathcal{H} \subseteq \mathbb{R}^d$ is a $(1+\epsilon)$-approximation of MVEE($\mathcal{S}$), where $\mathcal{H}$ is given by (9) (see Refs. 18,23). Therefore, we analyze Algorithm 2 for $\mathcal{S}' \subseteq \mathbb{R}^{d+1}$.

At iteration i, we define a "trial" ellipsoid $\tilde{\mathcal{E}}^i := \tilde{\mathcal{E}}_{M^i,0} \subseteq \mathbb{R}^{d+1}$ (cf. (14)), where

$$M^i := \frac{1}{d+1}\Pi(u^i)^{-1}, \quad i = 0, 1, 2, \ldots. \tag{27}$$

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

$$Q^i := \frac{1}{d}\left(PU^iP^T - (Pu^i)(Pu^i)^T\right)^{-1}, \quad c^i := Pu^i, \quad i = 0,1,2,\ldots. \tag{28}$$

Furthermore, by (27), vol $\tilde{\mathcal{E}}^i = \eta' \det(M^i)^{-1/2} = \eta'(d+1)^{(d+1)/2} \det \Pi(u^i)^{1/2}$, where η' is the volume of the unit ball in $\mathbb{R}^{d+1}$. Therefore,

$$\log \text{vol } \tilde{\mathcal{E}}^i = \log \eta' + \frac{d+1}{2}\log(d+1) + \frac{1}{2}\log\det\Pi(u^i), \quad i = 0,1,2,\ldots. \tag{29}$$

Similarly to (20), we have

$$\log \text{vol } \mathcal{E}^i = \log \eta + \frac{d}{2}\log d + \frac{1}{2}\log\det\Pi(u^i), \quad i = 0,1,2,\ldots, \tag{30}$$

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 only on d.

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

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

We define

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

so that $\mathcal{S}' \subseteq \sqrt{1+\epsilon_i}\,\tilde{\mathcal{E}}^i$. ϵ_i can be viewed as a quality measure of iterate i. Combining (31) and (32), we obtain

$$\text{vol } \tilde{\mathcal{E}}^i \leq \text{vol MVEE}(\mathcal{S}') \leq (1+\epsilon_i)^{(d+1)/2}\text{vol } \tilde{\mathcal{E}}^i, \quad i = 0,1,2,\ldots. \tag{33}$$

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

$$\nu_i \leq \nu^* \leq (d+1)\log(1+\epsilon_i) + \nu_i, \quad i = 0, 1, 2, \ldots, \tag{34}$$

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

$$\nu_i := \log\det\Pi(u^i), \quad i = 0, 1, 2, \ldots, \tag{35}$$

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

By (32) and (27),

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

so that

$$\beta^i := \frac{\kappa^i - (d+1)}{(d+1)(\kappa^i - 1)} = \frac{\epsilon_i}{\kappa^i - 1}, \quad i = 0, 1, 2, \ldots. \tag{37}$$

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

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

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

$$\Pi(u^{i+1}) = (1-\beta^i)\Pi(u^i) + \beta^i\Pi(e_j) = \Pi(u^i)\left[(1-\beta^i)I + \beta^i\Pi(u^i)^{-1}\Pi(e_j)\right]. \tag{39}$$

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

$$\begin{aligned}
\log\det\Pi(u^{i+1}) &= \log\det\Pi(u^i) + d\log(1-\beta^i) + \log(1+\epsilon_i), \\
&= \log\det\Pi(u^i) - d\log\left(1+\frac{\epsilon_i}{d(1+\epsilon_i)}\right) + \log\left(1+\epsilon_i\right), \\
&\geq \log\det\Pi(u^i) - \frac{\epsilon_i}{1+\epsilon_i} + \log(1+\epsilon_i), \quad i=0,1,2,\ldots, \\
&\geq \log\det\Pi(u^i) + \begin{cases} \log 2 - \frac{1}{2} > 0 & \text{if } \epsilon_i \geq 1, \\ \frac{1}{8}\epsilon_i^2 & \text{if } \epsilon_i < 1. \end{cases}
\end{aligned} \tag{40}$$

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

Note that

$$\kappa^0 = \max_{k=1,\ldots,n}(q^k)^T\Pi(u^0)^{-1}q^k \leq \sum_{k=1}^{n}(q^k)^T\Pi(u^0)^{-1}q^k = n\ \mathrm{trace}(\Pi(e)^{-1}\Pi(e)) = n(d+1).$$

By (36), it follows that

$$\epsilon_0 \leq n-1. \tag{41}$$

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

$$\begin{aligned}
\nu_0 &> -\infty, && \text{(42a)} \\
\delta_i := \nu^* - \nu_i &\leq (d+1)\log(1+\epsilon_i), \quad i=0,1,\ldots, && \text{(42b)} \\
\pi_i := \nu_{i+1} - \nu_i &\geq \log(1+\epsilon_i) - \frac{\epsilon_i}{1+\epsilon_i}, \quad i=0,1,\ldots, && \text{(42c)} \\
\delta_0 = \nu^* - \nu_0 &\leq (d+1)\log n. && \text{(42d)}
\end{aligned}$$

Khachiyan's analysis of Algorithm 2 (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

$$k = O(d\log\delta_0), \tag{43}$$

which implies that $k = O(d(\log d + \log\log n))$ by (42d).

The second stage of Khachiyan's analysis consists of bounding the number of iterations to halve ϵ_i assuming $\epsilon_i \leq 1$. 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 2 needs to run until

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

in order to obtain a $(1+\epsilon)$-approximation to 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.

4.1.2 A Different Interpretation of Khachiyan's Algorithm

Our presentation of the analysis of Khachiyan's 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),

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

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 towards p^j, i.e.,

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

Similarly, by (28),

$$(Q^i)^{-1} = d(PU^iP^T - (Pu^i)(Pu^i)^T) = d\sum_{k=1}^{n} u_k(p^k - c^i)(p^k - c^i)^T,$$

where we used $\sum_{k=1}^{n} u_k = 1$ and $Pu^i = c^i$. By (38), it follows that

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

which implies that the next trial ellipsoid is obtained by "expanding" the current trial ellipsoid towards 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, Khachiyan's algorithm implicitly generates 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.

4.2 A Modification

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

The following theorem gives a complexity bound for Algorithm 3.

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

Algorithm 3 Outputs a $(1+\epsilon)$-approximation of MVEE($\mathcal{S}$)

Require: Input set of points $\mathcal{S} = \{p^1, \ldots, p^n\} \subseteq \mathbb{R}^d$, $\epsilon \in (0,1)$

1: Run Algorithm 1 on $\mathcal{S}$ to get output $\mathcal{X}_0$.

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.

3: Run Algorithm 2 on $\mathcal{S}$ starting with u^0.

Proof. By Lemma 3.1, Algorithm 1 returns $\mathcal{X}_0 \subseteq \mathcal{S}$ 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 1 applied to ($\mathbf{D}(\mathcal{X}_0)$), it follows from (42d) that

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

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

By Lemma 3.1, vol MVEE($\mathcal{S}$) $\leq d^{2d}$vol MVEE($\mathcal{X}_0$). Taking logarithms on both sides, it follows from (30) that

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

where u^* denotes the optimal solution of ($\mathbf{D}(\mathcal{S})$). 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 2, it follows from (42d) and (43) that Algorithm 3 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 2, we obtain the desired complexity result. □

4.3 A 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 only on d and ϵ, but not on n.

Theorem 4.3 *Let $\epsilon > 0$. For a given set $\mathcal{S} = \{p^1, \ldots, p^n\} \subseteq \mathbb{R}^d$ of n points, let u^f denote the final iterate returned by Algorithm 3 applied to $\mathcal{S}$. Let $\mathcal{X} := \{p^k \in \mathcal{S} : u^f_k > 0,\ k = 1, \ldots, n\}$. Then, $\mathcal{X}$ is an ϵ-core set of $\mathcal{S}$. Furthermore,*

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

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 3 has at most $2d$ positive components and at each iteration, at most one component becomes positive. Therefore,

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

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),

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

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

$$\text{vol } \tilde{\mathcal{E}}^f \leq \text{vol MVEE}(\mathcal{S}') \leq (1+\epsilon) \text{ vol } \tilde{\mathcal{E}}^f = \text{vol } \tilde{\mathcal{E}}, \tag{52}$$

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

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

$$\frac{1}{1+\epsilon}\text{vol } \tilde{\mathcal{E}} = \text{vol } \tilde{\mathcal{E}}^f \leq \text{vol MVEE}(\mathcal{X}'), \tag{53}$$

which, together with (52), implies that

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

Since lifting preserves the approximation factor, it follows from (51), (52), and (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 MVEE$(\mathcal{X})$ and to MVEE$(\mathcal{S})$. Therefore, $\mathcal{X}$ is an ϵ-core set of $\mathcal{S}$.

$\square$

Remark 1: The size of the core set $\mathcal{X}$ in Theorem 4.3 depends only on 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 2: The proof of Theorem 4.3 can be applied to Khachiyan's algorithm (i.e., Algorithm 2) as well and a core set can similarly be defined upon termination. However, Algorithm 2 uses an initial iterate all of whose components are positive. Therefore, for instances with $n \gg d$, Algorithm 2 will return $\mathcal{S}$ itself as a trivial core set. The reduction in the size of the core set is a consequence of using Algorithm 1 to obtain an initial iterate with a provably better lower bound on the optimal value of $(\mathbf{D}(\mathcal{S}))$.

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 only on 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. 31–35) and introduces, for the first time, the notion of core sets for minimum volume enclosing ellipsoids.

Since most applications of the MVEE problem have relatively small dimension d and 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 in 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.

For future work, we intend to explore practical implementations based on the idea of core sets. 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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