Approximate Minimum Volume Enclosing Ellipsoids Using Core Sets

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Introduction

The MVEE Problem: Given a set $S = \{p_1, \ldots, p_n\}$ of n points in $\mathbb{R}^d$, compute an ellipsoid of minimum volume enclosing S (a.k.a., the Löwner ellipsoid of S).

Remarks:

- The Löwner ellipsoid always exists and is unique.
- The center of the Löwner ellipsoid lies in the interior of $\mathrm{conv}(S)$, the convex hull of S. (Danzer, Laugwitz, and Lenz, 1957)

Applications

- ➢ Optimal Design
- ➢ Computational Geometry
- ➢ Integer Programming (Lenstra's volume algorithm)
- ➢ Computer Graphics
- ➢ Pattern Recognition
- ➢ Statistics
- ➢ Nondifferentiable Convex Optimization
- ➢ Khachiyan's Ellipsoid Algorithm, etc.

Related Problems

- Given a polytope $S = \{x \in \mathbb{R}^d : Ax \leq b\}$, compute a *maximum* volume inscribed ellipsoid (MVIE).
- The Löwner ellipsoid problem for $S = \{p_1, \ldots, p_n\} \subseteq \mathbb{R}^d$ can be reduced to (MVIE) in linear time. (Khachiyan and Todd, 1993)
- Both problems admit polynomial-time algorithms (to within arbitrary precision).

In contrast:

- Given a polytope $S = \{x \in \mathbb{R}^d : Ax \leq b\}$, computing a minimum volume enclosing ellipsoid is $\mathcal{NP}$-complete.
- Given $S = \{p_1, \ldots, p_n\} \subseteq \mathbb{R}^d$, computing a maximal volume inscribed ellipsoid for $\text{conv}(S)$ is $\mathcal{NP}$-complete.

Previous Work

- Gradient-descent type first-order algorithms (Titterington, 1975, 1978; Silvermann and Titterington, 1973; Khachiyan, 1996)
- (Second-order) interior-point algorithms (Khachiyan and Todd, 1993; Nesterov and Nemirovskii, 1994; Nemirovskii, 1997; Zhang, 1998; Zhang and Gao, 2001; Anstreicher, 2001; Sun and Freund, 2002)
- $\mathcal{O}(d^{O(d)}n)$ algorithms for fixed dimension d
  1. Randomized (Welzl, 1991; Matousék, Sharir, and Welzl, 1992)
  2. Deterministic (Chazelle and Matousék, 1993)

Motivation

- Admits a formulation as a nice convex optimization problem.
- Several applications require solution for huge data sets in relatively small dimensions ($n \approx 10^6 - 10^7$ and $d \approx 30$).
- Current solvers run out of memory quickly.
- We extend the previous core set approach of Kumar, Mitchell, and Yıldırım (2003) for the Minimum Enclosing Ball problem. ($\mathcal{O}(\frac{1}{\epsilon})$ core set size)
- We prove improved worst-case complexity results.

Preliminaries

- $S = \{p_1, \ldots, p_n\}$: input set consisting of n points in $\mathbb{R}^d$
- A (full-dimensional) ellipsoid $E_{Q,c}$ in $\mathbb{R}^d$:

$$E_{Q,c} = \{x \in \mathbb{R}^d : (x-c)^T Q(x-c) \leq 1\}$$

  $Q \in \mathbb{R}^{d \times d}$ is symmetric and positive definite, $c \in \mathbb{R}^d$ is the center of $E_{Q,c}$.
- Volume of an ellipsoid $E_{Q,c}$:

$$\text{vol } E_{Q,c} = B \text{ det } Q^{-\frac{1}{2}}$$

  B is the volume of the unit ball in $\mathbb{R}^d$.
- MVEE(S): Minimum volume enclosing ellipsoid of S
- Fritz John inequality:

$$\frac{1}{d}\text{MVEE}(S) \subseteq \text{conv}(S) \subseteq \text{MVEE}(S)$$

Core Sets

(cf. Bădoiu, Har-Peled, Indyk, 2002)

- An ellipsoid $E_{Q,c} \supseteq S$ is said to be a $(1+\epsilon)$-approximation to the MVEE(S) if

$$\text{vol } E_{Q,c} \leq \text{ vol } (1+\epsilon) \text{ MVEE}(S) = (1+\epsilon)^d \text{ vol MVEE}(S).$$

- A set $X \subseteq S$ is called a *core set for S* if $S \subseteq E_{Q,c} := (1+\epsilon)\text{MVEE}(X)$. (i.e., $E_{Q,c}$ is a $(1+\epsilon)$-approximation to the MVEE(S).)

A Snapshot of Main Results

- There exists a core set $X \subseteq S$ with

$$|X| = \alpha = \mathcal{O}(d \log d + \tfrac{d}{\epsilon}) .$$

- MVEE(S) can be computed in

$$\mathcal{O}(nd^2\alpha + \alpha^{4.5} \log \tfrac{\alpha}{\epsilon})$$

  arithmetic operations.
- This is an improvement over the previously known results for large scale instances with $n \gg d$ and reasonably small values of $\epsilon > 0$.

Optimization Formulation

- **Assumption:** $S = \{p_1, \ldots, p_n\}$ is affinely independent.

$$\text{(D(S))} \quad \max_u \quad \log\det\left(\sum_{i=1}^n u_i \begin{bmatrix} p_i \\ 1 \end{bmatrix} \begin{bmatrix} p_i^T & 1 \end{bmatrix}\right)$$

$$\text{s.t.} \quad \sum_{i=1}^n u_i = 1$$

$$u \geq 0,$$

$u \in \mathbb{R}^n$ is the decision variable.

- This is the dual problem to that of computing the Löwner ellipsoid for the *lifted* point set in $\mathbb{R}^{d+1}$.

Relating MVEE(S) to D(S)

Lemma 1. Let $S = \{p_1, \ldots, p_n\}$ and $P = [p_1, \ldots, p_n] \in \mathbb{R}^{d \times n}$. If $u^* \in \mathbb{R}^n$ is an optimal solution of (D(S)), then $\text{MVEE}(S) = E_{Q,c}$, where

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

Algorithm 1

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Require: S = {p_1, ..., p_n} ⊆ R^d, ε > 0, X_0 ⊆ S
k ← 0
loop
    Compute MVEE(X_k) = E_{Q,c} using Khachiyan's algorithm.
    if S \ (1 + ε)E_{Q,c} = ∅ then
        Return MVEE(X_k), X_k
    else
        j ← arg max_{i=1,...,n} (c − p_i)^T Q(c − p_i).
    end if
    X_{k+1} ← X_k ∪ {p_j},  k ← k + 1.
end loop
```

Analysis of Algorithm 1

- Initialization step (Choice of X_0)
- Computation of MVEE(X_i), $i = 0, 1, \ldots$
- A lower bound on the increase in vol MVEE(X_i) at each iteration
- An upper bound on the number of iterations (i.e., number of core set updates)

Initialization

Lemma 2. There exists a subset $X_0 \subseteq S$ with $|X_0| = 2d$ such that

$$\text{volMVEE}(S) \leq \mathcal{O}(d^d) \text{ vol MVEE}(X_0).$$

The set X_0 can be calculated in $\mathcal{O}(nd^2)$ time.

Remark: The algorithm is based on those of Betke and Henk, 1993, and Matousék, 2001. The proof uses their results in conjunction with John's inequality.

Subproblems

Theorem 1. [Khachiyan, 1993] For a given set X of k points in $\mathbb{R}^d$ and $\delta > 0$, there exists an algorithm that computes an ellipsoid $E_{Q,c} \supseteq S$ such that $\mathrm{vol}(E_{Q,c}) \leq (1+\delta)\ \mathrm{vol}\ \mathrm{MVEE}(S)$, in $\mathcal{O}(k^{3.5} \log(\frac{k}{\delta}))$ operations.

Remark: The complexity result (in the real-number model) is based on a clever combination of first-order and second-order interior-point algorithms. This is currently the best known complexity result.

Expansion

Theorem 2. Let $\epsilon \in (0, 1/3)$. Then,

$$\text{vol MVEE}(X_{i+1}) \geq \text{vol MVEE}(X_i) e^{C\epsilon^2}$$

for some constant $C > 0$.

"Proof":

- Construct a feasible solution u' for (D(X_{i+1})) by using the optimal solution u of (D(X_i)).
- u' yields a lower bound on the optimal value of (D(X_{i+1})).

Core Set Size

Theorem 3. Let $\epsilon \in (0, 1/3)$. There exists a core set $X \subseteq S$ such that

$$|X| = \mathcal{O}\left(\frac{d \log d}{\epsilon^2}\right) .$$

Remark: This result follows from Lemma 2 (initial core set result) and Theorem 2 (expansion). Note the core set size.

Refined Core Set Size

Require: Input: $S \subset \mathbb{R}^d$, $\epsilon = 2^{-m}$, $X_0 \subset S$

1: **for** $i = 1$ to m **do**

2: Call Algorithm 1 with input S, $\epsilon = 2^{-i}$, X_{i-1}

3: $X_i \leftarrow$ the output core-set

4: **end for**

5: Return MEB$(X_m), X_m$

Theorem 3. Let $\epsilon = 2^{-m} \in (0, 1/3)$. Then, the algorithm returns a core set X such that $|X| = \mathcal{O}(d \log d + \frac{d}{\epsilon})$.

Complexity Result

Theorem 4. Algorithm 1 computes a $(1+\epsilon)$-approximation to the minimum volume enclosing ellipsoid of a given point set $S = \{p_1, \ldots, p_n\} \subseteq \mathbb{R}^d$ in at most

$$\mathcal{O}(nd^2\alpha + \alpha^{4.5} \log \tfrac{\alpha}{\epsilon})$$

operations, where

$$\alpha := \mathcal{O}(d \log d + \tfrac{d}{\epsilon})$$

denotes the size of the core set $X \subseteq S$.

Extensions: Balls and Ellipsoids

- Lemma 2 (core set initialization) extends and X_0 can be computed in $\mathcal{O}(nd^2)$ and $\mathcal{O}(nd^3)$ operations for balls and ellipsoids, respectively.
- Checking stopping conditions is a nontrivial problem.
- Stopping conditions be cast as a semidefinite feasibility problem ($\mathcal{O}(d^4)$ algorithm for each ball or ellipsoid, Porkolab and Khachiyan, 1997).
- The original problem can be cast as a semidefinite programming problem and solved in polynomial time. (Ben-Tal and Nemirovskii, 2001)

Conclusions and Future Directions

- A new algorithm to compute MVEE (S) with an improved worst-case complexity.
- Computational experiments are underway.
- Improved core set results?
- Optimized implementation (e.g., warm-starts, stopping condition, data structures, platform, etc.)
- Practical algorithms for balls and ellipsoids?
- Core set results for other geometric optimization problems?