Exact Analysis of Optimal Configurations in Radii Computations

(Extended abstract)

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Abstract

We propose a novel characterization of (radii-) minimal projections of polytopes onto j-dimensional subspaces. Applied on simplices this characterization allows to reduce the computation of an outer radius to a computation in the circumscribing case or to the computation of an outer radius of a lower-dimensional simplex. This allows to close a gap in the knowledge on optimal configurations in radii computations, such as determining the radii of smallest enclosing cylinders of regular simplices in general dimension.

1 Introduction

Radii computations of the following form occur in many applications in computer vision, robotics, computational biology, and massive data set analysis (see [7] and the references therein). Let $\mathcal{L}_{j,n}$ be the set of all j-dimensional linear subspaces (hereafter j-spaces) in *n*-dimensional Euclidean space \mathbb{E}^n . The *outer j*radius $R_j(C)$ of a convex body $C \subset \mathbb{E}^n$ is the radius of the smallest enclosing j-ball in an optimal orthogonal projection of C onto a j-space $J \in \mathcal{L}_{j,n}$, where the optimization is performed over $\mathcal{L}_{j,n}$. The optimal projections are called R_i -minimal projections. See $[1, 5, 10]$ for exact algebraic algorithms, $[8, 11, 14]$ for approximation algorithms, and [3, 7] for the computational complexity. In this paper we show the following new characterization of optimal projections:

Theorem 1 *Let* $1 \leq j \leq n \leq m$ *and* $P =$ $conv\{v^{(1)}, \ldots, v^{(m)}\} \subset \mathbb{E}^n$ be an *n*-polytope. Then *one of the following is true.*

- *a)* In every R_i -minimal projection of P there exist n+1 *affinely independent vertices of* P *which are projected onto the minimal enclosing* j*-sphere.*
- *b*) *j* ≥ 2 and $R_j(P) = R_{j-1}(P \cap H)$ for some hyper*plane* $H = \text{aff}\{v^{(i)} : i \in I\}$ *with* $I \subset \{1, ..., m\}$ *.*

If $i = 1$ *or if P is a regular simplex then always case a) holds. Moreover, the number* ν *of affinely indepen-* *dent vertices projected onto the minimal enclosing* j*sphere is at least* $n-j+2$ *and there exists a (v-1)-flat* F such that $R_j(P) = R_{j+\nu-n-1}(P \cap F)$. The bound $n - j + 2$ *is best possible.*

Theorem 1 allows to reduce the computation of an outer radius of a simplex to the computation in the circumscribing case or to the computation of an outer radius of a facet of the simplex. Reductions of smallest enclosing cylinders to circumscribing cylinders are used in exact algorithms as well as for complexity proofs (see, e.g., [1] and [7]), and have previously been given only for $j \in \{1, n\}$ as well as for dimension 3. Theorem 1 generalizes and unifies these results.

The characterization provides effective means for the analysis of optimal configurations in radii computations (for general dimension a known difficult task). As an example, we reduce the computation of the outer $(n-1)$ -radius of a regular simplex to the following optimization problem of symmetric polynomials in n variables:

$$
\begin{array}{rcl}\n\min & \sum_{i=1}^{n+1} s_i^4 & \text{s.t.} & \sum_{i=1}^{n+1} s_i^3 & = & 0, \\
\sum_{i=1}^{n+1} s_i^2 & = & 1, \text{ and } \sum_{i=1}^{n+1} s_i & = & 0.\n\end{array} \tag{1}
$$

The system is solved by reducing it to an optimization problem in six variables with additional integer constraints, leading to the following result.

Theorem 2 *Let* $n \geq 2$ *and* T_1^n *be a regular simplex in* \mathbb{E}^n *with edge length 1. Then*

$$
R_{n-1}(T_1^n) = \begin{cases} \sqrt{\frac{n-1}{2(n+1)}} & \text{if } n \text{ is odd,} \\ \frac{2n-1}{2\sqrt{2n(n+1)}} & \text{if } n \text{ is even.} \end{cases}
$$

The case *n* odd has already been settled independently by Pukhov [9] and Weißbach [12] who both left open the even case. There also exists a later paper on $R_{n-1}(T_1^n)$ for even n [13], but as pointed out in [1] the proof contained a crucial error. Thus Theorem 2 (re-)completes the determination of the sequence of outer *j*-radii of regular simplices $[9]$. ¹

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¹All omitted proofs as well as further analysis of the problems can be found in the full paper [2].

2 Preliminaries

Throughout the paper we work in Euclidean space \mathbb{E}^n , i.e., \mathbb{R}^n with the usual scalar product $x \cdot y$ and norm $||x|| = (x \cdot x)^{1/2}$. \mathbb{B}^n and \mathbb{S}^{n-1} denote the (closed) unit ball and unit sphere, respectively. For a set $A \subset \mathbb{E}^n$, the linear, affine, and convex hull of A are denoted by $\text{lin}(A)$, aff (A) , and conv (A) , respectively.

A set $C \subset \mathbb{E}^n$ is called a *body* if it is compact, convex and contains interior points. Accordingly, we always assume that a polytope $P \subset \mathbb{E}^n$ is fulldimensional (unless otherwise stated). Let $1 \leq j \leq n$. A j-flat F (an affine subspace of dimension j) is perpendicular to a hyperplane H with normal vector h if h and F are parallel. For $p, p' \in \mathbb{E}^n$ and subspaces $E \in \mathcal{L}_{j,n}, E' \in \mathcal{L}_{j',n}, \text{ a } j\text{-flat } F = p + E \text{ and a } j'\text{-flat}$ $F' = p' + E'$ are parallel if $E \cup E' = \text{lin}(E \cup E')$. A jcylinder is a set of the form $J+\rho\mathbb{B}^n$ with an $(n-j)$ -flat *J* and $\rho > 0$. Let $1 \leq j \leq k \leq n$. If $C' \subset \mathbb{E}^n$ is a compact, convex set whose affine hull F is a k -flat then $R_j(C')$ denotes the radius of a smallest enclosing jcylinder \mathcal{C}' relative to F, i.e., $\mathcal{C}' = J' + R_j(C')(\mathbb{B}^n \cap F)$ with a $(k - j)$ -flat $J' \subset F$.

A simplex conv $\{v^{(1)}, \ldots, v^{(n+1)}\}$ (with affinely independent $v^{(1)}, \ldots, v^{(n+1)} \in \mathbb{E}^n$) is *regular* if all its vertices are equidistant. Whenever a statement is invariant under orthogonal transformations and translations we denote by T^n the regular simplex in \mathbb{E}^n with edge length $\sqrt{2}$. Let $\mathcal{H}_{\alpha}^{n} = \{x \in \mathbb{E}^{n+1} : \sum_{i=1}^{n+1} x_i =$ α . Then the *standard embedding* \mathbf{T}^n of T^n is defined by $\mathbf{T}^n = \text{conv}\left\{e^{(i)} \in \mathbb{E}^{n+1} : 1 \leq i \leq n+1\right\} \subset \mathcal{H}_1^n,$ where $e^{(i)}$ denotes the *i*-th unit vector in \mathbb{E}^{n+1} . By $\mathcal{S}^{n-1} := \mathbb{S}^n \cap \mathcal{H}_0^n$ we denote the set of unit vectors parallel to \mathcal{H}_1^n . A *j*-cylinder $\mathcal C$ containing some simplex S is called a circumscribing j-cylinder of S if all the vertices of S are contained in the boundary of \mathcal{C} .

3 Minimal and circumscribing j**-cylinders**

The minimal enclosing ball B of a polytope $P \subset \mathbb{E}^n$ may contain only few vertices of P on its boundary, but in cases where less than $n + 1$ vertices of P are contained in the boundary of B , there exists a hyperplane H such that $P \cap \text{bd}(B) \subset H$ and the center of B is contained in H . Then the smallest enclosing ball of P and the smallest enclosing ball of $P \cap H$ relative to H have the same radius. In [6] the following characterization for the minimal enclosing 1-cylinder (two parallel hyperplanes defining the width of the polytope) is given:

Proposition 3 *Any minimal enclosing 1-cylinder of a polytope* $P \subset \mathbb{E}^n$ *contains at least* $n + 1$ *affinely independent vertices of* P *on its boundary.*

We provide a characterization of the possible configurations of minimal enclosing j-cylinders of polytopes, unifying and generalizing the above statements.

Lemma 4 Let $P = \text{conv}\{v^{(1)}, \ldots, v^{(m)}\}$ be a poly*tope in* \mathbb{E}^n , $1 \leq j \leq n-1$, and *J be an* $(n-j)$ *-flat* such that $\mathcal{C} = \tilde{J} + R_j(P)\mathbb{B}^n$ *is a minimal enclosing j*-cylinder of P. Then for every $I \subset \{1, \ldots, m\}$ such *that* $\{i : v^{(i)} \in bd(\mathcal{C})\} \subset I$ *and* $H_I := aff\{v^{(i)} : i \in$ I} is of affine dimension $n-1$, J is parallel to H_I .

Proof. Suppose that there exists a hyperplane $H :=$ H_I of this type with J not parallel to H. Let \bar{n} := $|\{v^{(i)} \in H : 1 \leq i \leq m\}|$. Without loss of generality $H = \{x \in \mathbb{E}^n : x_n = 0\}$ and $I = \{v^{(1)}, \ldots, v^{(\bar{n})}\}.$ Hence, $v^{(\bar{n}+1)},\ldots,v^{(\bar{m})} \notin H \cup \mathrm{bd}(C)$.

It suffices to consider the case that J is not perpendicular to H. Let $p, s^{(1)}, \ldots, s^{(n-j)} \in \mathbb{E}^n$ such that $J = p + \ln\{s^{(1)}, \ldots, s^{(n-j)}\}$. Since J is not parallel to H, we can assume $p = 0 \in J \cap H$, $s_n^{(1)} = \cdots = s_n^{(n-j-1)} = 0$ and $s_n^{(n-j)} > 0$. For every $s'_n \in (0, s_n^{(n-j)})$ and $s' := (s_1^{(n-j)}, \dots, s_{n-1}^{(n-j)}, s'_n) \in \mathbb{E}^n$ let $J' = p + \ln\{s^{(1)}, \ldots, s^{(n-j-1)}, s'\}$. Since J and H are not perpendicular we obtain $J \neq J'$, and because $v^{(1)},\ldots,v^{(\bar{n})} \in H$ that

$$
dist(v^{(i)}, J') \leq dist(v^{(i)}, J), \quad 1 \leq i \leq \bar{n},
$$
 (2)

where $dist(\cdot, \cdot)$ denotes the Euclidean distance. In (2) , "<" holds whenever $v^{(i)} \notin K := J^{\perp} \cap H$. Obviously, $\dim(K) = j - 1$. If none of the $v^{(i)}$ lies in $K \cap \mathrm{bd}(\mathcal{C})$ then, by choosing s'_n sufficiently close to $s_n^{(n-j)}$, all vertices of P lie in the interior of $\mathcal{C}' = J' + R_i(P)\mathbb{B}^n$, a contradiction to the minimality of C . Hence, there must be some vertex of P in $K \cap \mathrm{bd}(\mathcal{C})$. Let $\overline{k} := |\{v^{(i)} \in K \cap \mathrm{bd}(\mathcal{C}) : 1 \leq i \leq m\}|.$ We can assume that $v^{(1)}, \ldots, v^{(k)} \in K \cap \text{bd}(\mathcal{C})$. Let $F := \text{conv}\{v^{(1)}, \ldots, v^{(\bar{k})}\}\$ and $k := \dim F$. Suppose $F \cap J = \emptyset$. We have shown above that for sufficiently small s'_n the rotation from J to J' keeps all vertices within the *j*-cylinder \mathcal{C}' and $v^{(1)}, \ldots, v^{(k)}$ are the only vertices on $\text{bd}(\mathcal{C}')$. Let J'' be a translate of J' with $dist(J'', F) < dist(J', F)$, and J'' sufficiently close to J' to keep $v^{(\bar{k}+1)},\ldots,v^{(\hat{m})}$ within the interior of $\mathcal{C}'' = J'' + R_j(P)\mathbb{B}^n$. Then all vertices of P lie in the interior of \mathcal{C}'' , again a contradiction.

It follows that $F \cap J \neq \emptyset$, and since $F \subset K = J^{\perp} \cap H$ that $F \cap J = p = 0$. Since $dist(p, v^{(i)}) = R_i(P)$ for all $i \in \{1, \ldots, \bar{k}\}\$ and since $p \in F$, it follows that p is the unique center of the smallest enclosing k-ball of F. Let J''' result from J' by rotating J' around the origin towards a direction in $\mathbb{R}^n \setminus \bigcup_{i=1}^{\bar{k}} (v^{(i)})^{\perp}$). For $i \in \{1, \ldots, \bar{k}\}$ the property $dist(v^{(i)}, J) = dist(v^{(i)}, J') = dist(v^{(i)}, p)$ implies $dist(v^{(i)}, J''') < dist(v^{(i)}, J')$. By keeping the rotation sufficiently small, $v^{(\tilde{k}+1)}, \ldots, v^{(m)}$ remain in the interior of $\mathcal{C}''' = J''' + R_j(P)\mathbb{B}^n$. Now, all vertices lie in the interior of \mathcal{C}''' , once more a contradiction. \Box

Lemma 5 Let $P = \text{conv}\{v^{(1)}, \ldots, v^{(m)}\}$ be a poly*tope in* \mathbb{E}^n , $1 \leq j \leq n$, and *J be an* $(n - j)$ *-flat* such that $C = J + R_j(P) \mathbb{B}^n$ is a minimal enclos*ing* j*-cylinder of* P*. If there exists a hyperplane* $H_I = \text{aff}\{v^{(i)} : i \in I\}$ which is parallel to J, then *one of the following holds:*

a) There exists a vertex $v^{(i)} \notin H_I$ that lies on the *boundary of* C*; or*

b)
$$
j \ge 2
$$
, $J \subset H_I$, and $R_j(P) = R_{j-1}(P \cap H_I)$.

Proof. By Proposition 3, for $j = 1$ always a) holds; so let $j \geq 2$, and suppose neither a) nor b) holds. Since b) does not hold there exist $(n-j)$ -flats parallel to J and closer to H_I , and since a) does not hold, for any such $(n-j)$ -flat J', such that all vertices $v^{(i)} \notin H_I$ stay within \mathcal{C} , the distances from the vertices $v^{(i)}$, $i \in$ I, to J' are strictly smaller than their distances to J . Hence $\mathcal C$ cannot be a minimal enclosing cylinder. \Box

In the case that P is a simplex, the proof can be carried out more explicitly: Let $P^{(n+1)}$ be the facet of P not including the vertex $v^{(n+1)}$. Suppose that J is parallel to $P^{(n+1)}$, that $P^{(n+1)} \subset H := \{x \in \mathbb{E}^n :$ $x_n = 0$, and that $v_n^{(n+1)} > 0$. Let $p \in J$. Since $v_n^{(n+1)} > 0$ it follows $p_n \geq 0$ and obviously

$$
R_j(P) \ge v_n^{(n+1)} - p_n. \tag{3}
$$

On the other hand, since J is parallel to $P^{(n+1)}$,

$$
R_j(P)^2 = R_{j-1}^2(P^{(n+1)}) + p_n^2.
$$
 (4)

Let $p_n^* = ((v_n^{(n+1)})^2 - R_{j-1}^2(P^{(n+1)}))/2v_n^{(n+1)}$ be the unique minimal solution for p_n to (3) and (4). Due to $p_n \geq 0$, we obtain $p_n = \max\{0, p_n^*\}$. Now, we see that case a) holds if $p_n = p_n^*$ and case b) if $p_n = 0$.

If the number ν of affinely independent vertices of P lying on the boundary of $\mathcal C$ is at most n, it follows from Lemma 4 and 5 that case b) of Theorem 1 must hold. Moreover, if $\nu \leq n-1$ we can apply these lemmas on the lower-dimensional polytope $P \cap H_I$ with H_I as in Lemma 5. This argument can be iterated. If during this iteration the outer 1-radius of a polytope P' has to be computed, then by Proposition 3 the minimal enclosing 1-cylinder touches at least $\dim(P') + 1$ affinely independent vertices. From the same iterative argument it follows that $R_j(P) = R_{j+\nu-n-1}(P \cap F)$ for some $(\nu - 1)$ -flat F.

Suppose $S = \text{conv}\lbrace v^{(1)}, \ldots, v^{(n+1)} \rbrace$ is a simplex in \mathbb{E}^n , and \bar{J} an $(n - j)$ -flat, such that

$$
dist(v^{(1)}, J) = \cdots = dist(v^{(n-j+2)}, J)
$$

= $R_1(\text{conv}\{v^{(1)}, \dots, v^{(n-j+2)}\})$
> $dist(v^{(n-j+3)}, J)$
 $\geq \cdots \geq dist(v^{(n+1)}, J).$

Then $R_i(S) = R_1(\text{conv}\{v^{(1)}, \ldots, v^{(n-j+2)}\})$ and n $j + 2$ vertices are situated on the boundary of the minimal enclosing j-cylinder.

The last point which remains to proof Theorem 1 is that every minimal enclosing j-cylinder of the regular simplex T^n is circumscribing. Due to Proposition 4 it suffices to show that p_n^* is positive for all $1 \leq j \leq n-1$, showing that b) in Lemma 5 never holds for T^n . We omit the details and refer to the full paper [2].

4 Reduction to an algebraic optimization problem

In this section, we provide an algebraic formulation for a minimal circumscribing j-cylinder $J + \rho(\mathbb{B}^{n+1} \cap$ \mathcal{H}_0^n of the regular simplex \mathbf{T}^n . Let $J = p +$ $\lim_{s \to s} \{s^{(1)}, \ldots, s^{(n-j)}\}$ with pairwise orthogonal (p.o.) $s^{(1)},\ldots,s^{(n-j)}\in\mathcal{S}^{n-1}$, and p be contained in the orthogonal complement of $\text{lin}\lbrace s^{(1)},\ldots,s^{(n-j)}\rbrace$. The projection P of a vector $z \in \mathcal{H}_1^n$ onto the orthogonal complement of $\text{lin}\lbrace s^{(1)},\ldots,s^{(n-j)}\rbrace$ (relative to \mathcal{H}_1^n) can be written as $P(z) = (I - \sum_{k=1}^{n-j} s^{(k)} (s^{(k)})^T) z$, where I denotes the identity matrix. Using the convention $x^2 := x \cdot x$, the computation of the square of R_i for a polytope with vertices $v^{(1)}, \ldots, v^{(m)}$ (embedded in \mathcal{H}_1^n) can be expressed as

(i) s.t.
$$
(p - Pv^{(i)})^2 \leq \rho^2
$$
,
\n(ii) $p \cdot s^{(k)} = 0$,
\n(iii) $s^{(1)}, \ldots, s^{(n-j)} \in S^{n-1}$, p.o.,
\n(iv) $p \in \mathcal{H}_1^n$,

where $i = 1, \ldots, m$ and $k = 1, \ldots, n - j$. In the case of \mathbf{T}^n , (i) can be replaced by

(i')
$$
\left(p - e^{(i)} + \sum_{k=1}^{n-j} s_i^{(k)} s^{(k)}\right)^2 = \rho^2,
$$

where the equality sign follows from Theorem 1. By (ii) and $s^{(k)} \in \mathcal{S}^{n-1}$, (i') can be simplified to

(i")
$$
p^2 - \rho^2 = \sum_{k=1}^{n-j} (s_i^{(k)})^2 + 2p_i - 1
$$
.

Summing over all *i* gives $(n+1)(p^2 - \rho^2) = (n-j)+2 (n+1)$, i.e., $p^2 - \rho^2 = \frac{1-j}{n+1}$. We substitute this value into (i") and obtain $p_i = \frac{1}{2} \left(\frac{n-j+2}{n+1} - \sum_{k=1}^{n-j} (s_i^{(k)})^2 \right)$. Hence, all the p_i can be replaced in terms of the $s_i^{(k)}$,

$$
\rho^2 = \frac{(2 + (n - j))(2 - (n - j))}{4(n + 1)} \n+ \frac{1}{4} \sum_{i=1}^{n+1} \left(\sum_{k=1}^{n-j} (s_i^{(k)})^2 \right)^2 + \frac{j-1}{n+1}, \quad (5) \np \cdot s^{(k)} = -\frac{1}{2} \sum_{i=1}^{n+1} \sum_{k'=1}^{n-j} (s_i^{(k')})^2 s_i^{(k)}.
$$

We arrive at the following characterization of the minimal enclosing j-cylinders:

Theorem 6 Let $1 \leq j \leq n$. A set of vectors $s^{(1)},\ldots,s^{(n-j)} \in \mathcal{S}^{n-1}$ spans the underlying $(n-j)$ j)*-dimensional subspace of a minimal enclosing* j*cylinder of* $\mathbf{T}^n \subset \mathcal{H}_1^n$ *if and only if it is an optimal solution of the problem*

$$
\min \sum_{i=1}^{n+1} \left(\sum_{k=1}^{n-j} (s_i^{(k)})^2 \right)^2
$$
\n
$$
\text{s.t.} \sum_{i=1}^{n+1} \sum_{\substack{k'=1 \ k'=1}}^{n-j} (s_i^{(k')})^2 s_i^{(k)} = 0,
$$
\n
$$
s^{(1)}, \dots, s^{(n-j)} \in \mathcal{S}^{n-1}, \quad p.o.,
$$

where $k = 1, \ldots, n - j$.

In case $j = n - 1$ the previous program reduces to (1). By (5), in order to prove $R_{n-1}(T^n) = (2n 1)/(2\sqrt{n(n+1)})$ for even n, we have to show that the optimal value of (1) is $1/n$. We apply the following statement from [1].

Proposition 7 *Let* $n \geq 2$ *. The direction vector* $(s_1, \ldots, s_{n+1})^T$ *of any extreme circumscribing* $(n-1)$ *cylinder of* \mathbf{T}^n *satisfies* $|\{s_1,\ldots,s_{n+1}\}| \leq 3$ *.*

Using Proposition 7, (1) can be written as the following polynomial optimization problem in six variables with additional integer conditions.

$$
\begin{array}{rcl}\n\text{min } k_1 s_1^4 + k_2 s_2^4 + k_3 s_3^4 \\
\text{(i) s.t.} & k_1 s_1^3 + k_2 s_2^3 + k_3 s_3^3 = 0, \\
\text{(ii) } & k_1 s_1^2 + k_2 s_2^2 + k_3 s_3^2 = 1, \\
\text{(iii) } & k_1 s_1 + k_2 s_2 + k_3 s_3 = 0, \\
\text{(iv) } & k_1 + k_2 + k_3 = n+1,\n\end{array}\n\tag{6}
$$

$$
s_1, s_2, s_3 \in \mathbb{R}, \quad k_1, k_2, k_3 \in \mathbb{N}_0 \, .
$$

Since the odd case of Theorem 2 is well-known [9, 12], we assume from now on that n is even.

For $k_3 = 0$ the equality constraints in (6) immediately yield $k_1 = k_2 = (n + 1)/2 \notin \mathbb{N}$, and similarly, for $s_2 = s_3$ we obtain $k_1 = k_2 + k_3 = (n+1)/2 \notin \mathbb{N}$. Hence, we can assume that s_1 , s_2 , and s_3 are distinct and $k_1, k_2, k_3 \geq 1$. Moreover, for $s_3 = 0$ the resulting optimal value is $1/n$ which will turn out to be the optimal solution. Finally, by (iii), not all of the s_i have the same sign. Hence it suffices to show that for $s_1 < 0$ and $s_3 > s_2 > 0$ every admissible solution to the constraints of (6) has value at least $1/n$.

The linear system in k_1, k_2, k_3 defined by (i), (ii), and (iii) is regular and can be solved for k_1, k_2, k_3 :

$$
k_1 = \frac{s_2 + s_3}{-s_1(s_2 - s_1)(s_3 - s_1)}, \tag{7}
$$

$$
k_2 = \frac{s_1 + s_3}{s_2(s_2 - s_1)(s_3 - s_2)}, \tag{8}
$$

$$
k_3 = \frac{-(s_1 + s_2)}{s_3(s_3 - s_1)(s_3 - s_2)}.
$$
 (9)

Since all factors in the denominators are strictly positive, (8) and (9) imply in particular $s_1 + s_3 > 0$ and $s_1 + s_2 < 0.$

With (iv) in (6) we can express one of the s_i by the others, e.g. $s_2 = -\frac{s_1+s_3}{(n+1)s_1s_3+1}$, and using this it can be successively shown that $k_1 < (n+1)/2$. Thus by the integer condition $k_1 \leq n/2$, and it follows that for any admissible solution to the constraints of (6) the objective value is at least $1/n$ (for details see [2]). By our remark before Proposition 7 this completes the proof of Theorem 2.

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