

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

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

If $j = 1$ or if P is a regular simplex then always case a) holds. Moreover, the number ν of affinely independent

vertices projected onto the minimal enclosing j -sphere is at least $n-j+2$ and there exists a $(\nu-1)$ -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:

$$\min \begin{array}{l} \sum_{i=1}^{n+1} s_i^4 \\ \sum_{i=1}^{n+1} s_i^2 = 1, \end{array} \quad \text{s.t.} \quad \begin{array}{l} \sum_{i=1}^{n+1} s_i^3 = 0, \\ \sum_{i=1}^{n+1} s_i = 0. \end{array} \quad (1)$$

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 $\text{lin}(A)$, $\text{aff}(A)$, and $\text{conv}(A)$, 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 full-dimensional (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 $E \in \mathcal{L}_{j,n}$, $E' \in \mathcal{L}_{j',n}$, a j -flat $F = p + E$ and a j' -flat $F' = p' + E'$ are *parallel* if $E \cup E' = \text{lin}(E \cup E')$. A j -cylinder 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 j -cylinder C' relative to F , i.e., $C' = J' + R_j(C')(\mathbb{B}^n \cap F)$ with a $(k-j)$ -flat $J' \subset F$.

A simplex $\text{conv}\{v^{(1)}, \dots, v^{(n+1)}\}$ (with affinely independent $v^{(1)}, \dots, v^{(n+1)} \in \mathbb{E}^n$) 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 $\mathcal{H}_\alpha^n = \{x \in \mathbb{E}^{n+1} : \sum_{i=1}^{n+1} x_i = \alpha\}$. Then the *standard embedding* \mathbf{T}^n of T^n is defined by $\mathbf{T}^n = \text{conv}\{e^{(i)} \in \mathbb{E}^{n+1} : 1 \leq i \leq n+1\} \subset \mathcal{H}_1^n$, where $e^{(i)}$ denotes the i -th unit vector in \mathbb{E}^{n+1} . By $\mathbb{S}^{n-1} := \mathbb{S}^n \cap \mathcal{H}_0^n$ 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 $P = \text{conv}\{v^{(1)}, \dots, v^{(m)}\}$ be a polytope in \mathbb{E}^n , $1 \leq j \leq n-1$, and J be an $(n-j)$ -flat such that $\mathcal{C} = J + R_j(P)\mathbb{B}^n$ is a minimal enclosing j -cylinder of P . Then for every $I \subset \{1, \dots, m\}$ such that $\{i : v^{(i)} \in \text{bd}(\mathcal{C})\} \subset I$ and $H_I := \text{aff}\{v^{(i)} : i \in I\}$ 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 $I = \{v^{(1)}, \dots, v^{(\bar{n})}\}$. Hence, $v^{(\bar{n}+1)}, \dots, v^{(m)} \notin H \cup \text{bd}(\mathcal{C})$.

It suffices to consider the case that J is not perpendicular to H . Let $p, s^{(1)}, \dots, s^{(n-j)} \in \mathbb{E}^n$ such that $J = p + \text{lin}\{s^{(1)}, \dots, s^{(n-j)}\}$. Since J is not parallel to H , we can assume $p = 0 \in J \cap H$, $s_n^{(1)} = \dots = s_n^{(n-j-1)} = 0$ 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 $J' = p + \text{lin}\{s^{(1)}, \dots, s^{(n-j-1)}, s'\}$. Since J and H are not perpendicular we obtain $J \neq J'$, and because $v^{(1)}, \dots, v^{(\bar{n})} \in H$ that

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

where $\text{dist}(\cdot, \cdot)$ 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 $K \cap \text{bd}(\mathcal{C})$ then, by choosing s'_n sufficiently close to $s_n^{(n-j)}$, all vertices of P lie in the interior of $\mathcal{C}' = J' + R_j(P)\mathbb{B}^n$, a contradiction to the minimality of \mathcal{C} . Hence, there must be some vertex of P in $K \cap \text{bd}(\mathcal{C})$. Let $\bar{k} := |\{v^{(i)} \in K \cap \text{bd}(\mathcal{C}) : 1 \leq i \leq m\}|$. We can assume that $v^{(1)}, \dots, v^{(\bar{k})} \in K \cap \text{bd}(\mathcal{C})$. Let $F := \text{conv}\{v^{(1)}, \dots, v^{(\bar{k})}\}$ 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 $v^{(1)}, \dots, v^{(\bar{k})}$ are the only vertices on $\text{bd}(\mathcal{C}')$. Let J'' be a translate of J' with $\text{dist}(J'', F) < \text{dist}(J', F)$, and J'' sufficiently close to J' to keep $v^{(\bar{k}+1)}, \dots, v^{(m)}$ 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 $\text{dist}(p, v^{(i)}) = R_j(P)$ for all $i \in \{1, \dots, \bar{k}\}$ 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 $i \in \{1, \dots, \bar{k}\}$ the property $\text{dist}(v^{(i)}, J) = \text{dist}(v^{(i)}, J') = \text{dist}(v^{(i)}, p)$ implies $\text{dist}(v^{(i)}, J''') < \text{dist}(v^{(i)}, J')$. By keeping the rotation sufficiently small, $v^{(\bar{k}+1)}, \dots, v^{(m)}$ 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. \square

Lemma 5 *Let $P = \text{conv}\{v^{(1)}, \dots, v^{(m)}\}$ be a polytope in \mathbb{E}^n , $1 \leq j \leq n$, and J be an $(n-j)$ -flat*

such that $\mathcal{C} = J + R_j(P)\mathbb{B}^n$ is a minimal enclosing 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 \mathcal{C} ; or
- b) $j \geq 2$, $J \subset H_I$, 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. \square

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

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

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

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

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

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

Then $R_j(S) = R_1(\text{conv}\{v^{(1)}, \dots, v^{(n-j+2)}\})$ 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 $J = p + \text{lin}\{s^{(1)}, \dots, s^{(n-j)}\}$ with pairwise orthogonal (p.o.) $s^{(1)}, \dots, s^{(n-j)} \in \mathcal{S}^{n-1}$, and p be contained in the orthogonal complement of $\text{lin}\{s^{(1)}, \dots, s^{(n-j)}\}$. The projection P of a vector $z \in \mathcal{H}_1^n$ onto the orthogonal complement of $\text{lin}\{s^{(1)}, \dots, s^{(n-j)}\}$ (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_j for a polytope with vertices $v^{(1)}, \dots, v^{(m)}$ (embedded in \mathcal{H}_1^n) can be expressed as

$$\begin{aligned} &\min \rho^2 \\ \text{(i)} \quad &\text{s.t.} \quad (p - Pv^{(i)})^2 \leq \rho^2, \\ \text{(ii)} \quad & p \cdot s^{(k)} = 0, \\ \text{(iii)} \quad & s^{(1)}, \dots, s^{(n-j)} \in \mathcal{S}^{n-1}, \text{ p.o.}, \\ \text{(iv)} \quad & p \in \mathcal{H}_1^n, \end{aligned}$$

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

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

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

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

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 $s_i^{(k)}$,

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

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

Theorem 6 Let $1 \leq j \leq n$. A set of vectors $s^{(1)}, \dots, s^{(n-j)} \in \mathcal{S}^{n-1}$ spans the underlying $(n-j)$ -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

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

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

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 $(s_1, \dots, s_{n+1})^T$ of any extreme circumscribing $(n-1)$ -cylinder of \mathbf{T}^n satisfies $|\{s_1, \dots, s_{n+1}\}| \leq 3$.

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

$$\begin{aligned} \min \quad & k_1 s_1^4 + k_2 s_2^4 + k_3 s_3^4 \\ \text{(i) s.t.} \quad & k_1 s_1^3 + k_2 s_2^3 + k_3 s_3^3 = 0, \\ \text{(ii)} \quad & k_1 s_1^2 + k_2 s_2^2 + k_3 s_3^2 = 1, \\ \text{(iii)} \quad & k_1 s_1 + k_2 s_2 + k_3 s_3 = 0, \\ \text{(iv)} \quad & k_1 + k_2 + k_3 = n+1, \\ & s_1, s_2, s_3 \in \mathbb{R}, \quad k_1, k_2, k_3 \in \mathbb{N}_0. \end{aligned} \quad (6)$$

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 :

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

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

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

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. $s_2 = -\frac{s_1 + s_3}{(n+1)s_1 s_3 + 1}$, 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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