



INTRODUCTION

The problem of determining the optimal placement of a given number of points on the sphere \mathbb{S}^2 is a classic problem in geometry that has numerous applications to a wide variety of areas. In molecular science, the assumption of the valence-shell electron repulsion model is that the configuration of a given number of electron pairs in the valence shell of an atom is the one that maximizes the least distance between any pair (see, e.g., [5]). In Information Theory, the problem of determining optimal spherical codes involves optimizing some function of those points (see, e.g., [4]). In this paper, we determine the optimal placement of 5 vertices on the sphere so that the surface area of the convex hull of those points is maximized. This result proves a conjecture of Akkiraju [1] in the affirmative, and addresses a question of Kazakov [6] on the surface area entanglement measure in Quantum Information Theory.

MAIN RESULT

Consider a polytope P in \mathbb{R}^3 that has v vertices, e edges and f facets, and that the vertices of P lie in the unit sphere \mathbb{S}^2 . A special case of a result of Tóth [9, Thm. 2, p. 279] yields the inequality

$$S(P) \leq e \sin \frac{\pi f}{e} \left(1 - \cot^2 \frac{\pi f}{2e} \cot^2 \frac{\pi v}{2e} \right) =: G(v, e, f). \quad (1)$$

Thus, if $S(P) = G(v, e, f)$, then P must have maximum surface area among all polytopes inscribed in the ball with v vertices, e edges and f facets. In the case P_4 is a simplex, $v = f = 4$ and $e = 6$ and thus

$$S(P_4) \leq G(4, 6, 4) = 6 \sin \frac{2\pi}{3} \left(1 - \cot^4 \frac{\pi}{3} \right) = \frac{8}{\sqrt{3}} = 4.6188 \dots$$

On the other hand, the regular simplex P_4^* has surface area $S(P_4^*) = 8/\sqrt{3}$. Thus, P_4^* has maximum surface area among all polytopes with 4 vertices. More generally, a result of Tanner [8] implies that in any dimension $n \geq 2$, the regular simplex maximizes surface area.

In the case of polytopes P_6 with 6 vertices, then the possibilities for (v, e, f) are $(6, 9, 5)$, $(6, 10, 6)$, $(6, 11, 7)$ and $(6, 12, 8)$ (see, e.g., [3, Table II]). Checking cases, we find that $G(6, 12, 8)$ has the maximum value among the four possibilities. Hence,

$$S(P_6) \leq G(6, 12, 8) = 4\sqrt{3} = 6.9282 \dots$$

An elementary computation shows that the triangular bipyramid B_6^* with vertices $\pm e_1, \pm e_2, \pm e_3$ also has surface area $4\sqrt{3}$, and thus B_6^* is the optimal polytope with 6 vertices.

For the case of inscribed polytopes with 5 vertices, the answer seems to have been known for quite some time, at least numerically, but a proof was missing until now. Akkiraju [1, p. 753] asked for a proof that the surface area maximizer with 5 vertices is a bipyramid B_5^* with apexes at the north and south poles $\pm e_3$ and three vertices forming an equilateral triangle in the equator $\mathbb{S}^2 \cap e_3^\perp$. In our main result, we provide an affirmative answer to this question.

It turns out that up to graph isomorphism, there are only two types of polytopes with 5 vertices: the 5-pyramid with $(v, e, f) = (5, 8, 5)$ and the 5-bipyramid with $(v, e, f) = (5, 9, 6)$ (see, e.g., [3]). We have $G(5, 9, 6) > G(5, 8, 5)$ with $G(5, 9, 6) = \frac{9\sqrt{3}}{2} \left(1 - \frac{1}{3} \cot^2 \frac{5\pi}{18} \right) = 5.96495 \dots$ However, it is easy to check that

$$S(B_5^*) = 3\sqrt{15}/2 \approx 5.809 < G(5, 9, 6).$$

Thus, to prove that B_5^* is the optimal polytope, we will need a different argument. Our main result in [2] is the following.

Theorem 1. [2] *Among all polytopes with 5 vertices chosen from the sphere \mathbb{S}^2 , the bipyramid B_5^* with vertices $\pm e_3, e_1, (-\frac{1}{2}, \frac{\sqrt{3}}{2}, 0), (-\frac{1}{2}, -\frac{\sqrt{3}}{2}, 0)$ has maximal surface area, with $S(B_5^*) = \frac{3\sqrt{15}}{2}$.*

The proof of Theorem 1 uses several applications of the method of partial variation of Polya [7] and Lagrange multipliers.

As a follow-up question, we investigate the following problem.

Problem 1. *Determine the polytope inscribed in \mathbb{S}^2 with 5 facets that maximizes surface area.*

CONTACT INFORMATION

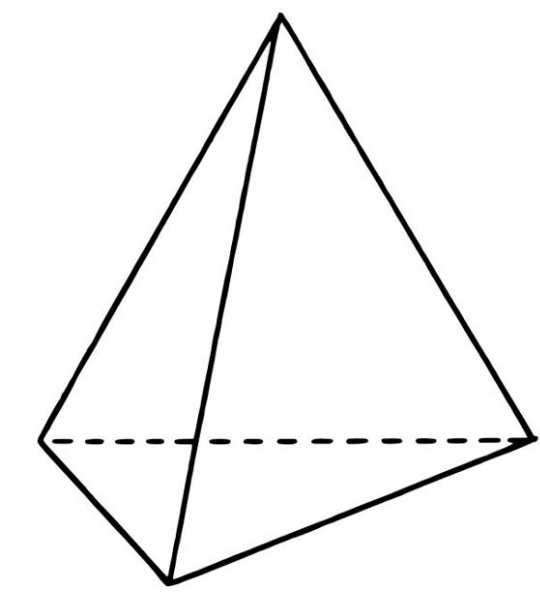
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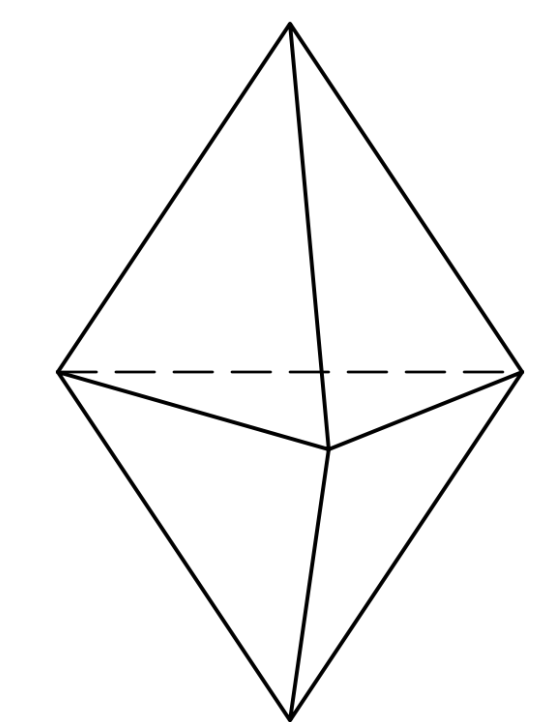
We would like to thank the PRISM program for its generous support.

OPTIMAL POLYTOPES

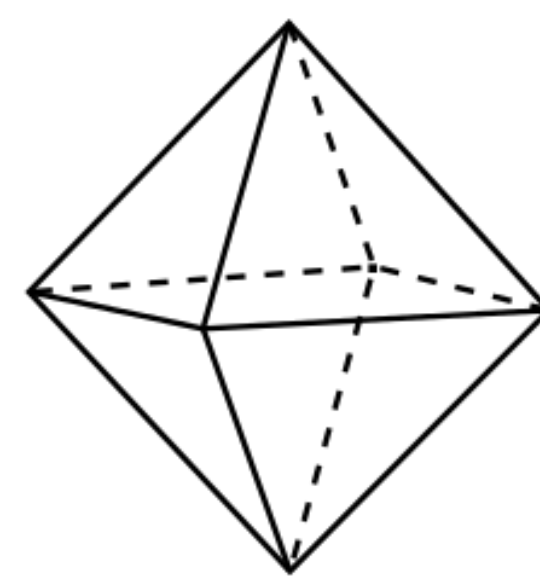
For 4 vertices, the optimal polytope is a regular simplex.



For 5 vertices, our main result says that the optimal polytope is a bipyramid with an equilateral triangle at the equator and apexes at the north and south poles.



For 6 vertices, the optimal polytope is an octahedron with a square at the equator and apexes at the north and south poles.



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