# McMaster University

### Advanced Optimization Laboratory



# **Title:** Small Kissing Polytopes

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AdvOL-Report No. 2024/1

November 2024, Hamilton, Ontario, Canada

#### SMALL KISSING POLYTOPES

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Dedicated to Tamás Terlaky on the occasion of his 70th birthday

#### ABSTRACT

A lattice (d, k)-polytope is the convex hull of a set of points in  $\mathbb{R}^d$  whose coordinates are integers ranging between 0 and k. We consider the smallest possible distance  $\varepsilon(d, k)$  between two disjoint lattice (d, k)-polytopes. We propose an algebraic model for this distance and derive from it an explicit formula for  $\varepsilon(2, k)$ . Our model also allows for the computation of previously intractable values of  $\varepsilon(d, k)$ . In particular, we compute  $\varepsilon(3, k)$ when  $4 \le k \le 8$ ,  $\varepsilon(4, k)$  when  $2 \le k \le 3$ , and  $\varepsilon(6, 1)$ .

#### 1. Introduction

The smallest possible distance between two disjoint lattice (d, k)-polytopes convex hulls of sets of points with integer coordinates in  $[0, k]^d$ —is a natural quantity in discrete geometry. This quantity, which we refer to as  $\varepsilon(d, k)$  in the sequel, is connected to the complexity of algorithms such as the linear minimization formulation by Gábor Braun, Sebastian Pokutta, and Robert Weismantel [4] of the von Neumann alternating projections algorithm [11]. It is also related to several notions that appear in optimization. For instance, the facial distance of a polytope P, studied by Javier Peña and Daniel Rodriguez [9] and by David Gutman and Javier Peña [6, 8], is the smallest possible distance between a face F of P and the convex hull of the vertices of P that are not contained in F. The vertex-facet distance of a polytope P, considered by Amir Beck and Shimrit Shtern [2], is the smallest possible distance between the affine hull of a facet F of P and a vertex of P that does not belong to F. The smallest possible vertex-facet distance of a lattice (d, 1)-simplex has been estimated by Noga Alon and Văn Vũ [1]. Another such notion is the pyramidal width of a finite set of points, investigated by Simon Lacoste-Julien and Martin Jaggi [7] and by Luis Rademacher and Chang Shu [10], which coincides with the facial distance of the convex hull of these points [9]. Gábor Braun, Alejandro Carderera, Cyrille Combettes, Hamed Hassani, Amin Karbasi, Aryan Mokhtari, and Sebastian Pokutta provide a comprehensive overview of these notions in [3].

Lower and upper bounds on  $\varepsilon(d, k)$  that are almost matching as d goes to infinity and a number of properties of this quantity as a function of d and k have been established by Shmuel Onn, Sebastian Pokutta, and two of the authors in [5]. The values of  $\varepsilon(2, k)$  when  $1 \le k \le 6$ , of  $\varepsilon(3, k)$  when  $1 \le k \le 3$ , of  $\varepsilon(4, 1)$ , and of  $\varepsilon(5, 1)$  have been computed as a consequence of these properties and are reported in [5] (see also the non-bolded entries in Table 1).

An algebraic model that allows for the computation of previously intractable values of  $\varepsilon(d, k)$  is developed in Section 2. More precisely,  $\varepsilon(d, k)$  is bounded by the smallest non-zero value of a certain algebraic fraction over a subset of the lattice points contained in the hypercube  $[-k, k]^{d^2}$ . Using this model, we provide the following formula for  $\varepsilon(2, k)$  in Section 3.

THEOREM 1.1: If k is greater than 1, then

$$\varepsilon(2,k) = \frac{1}{\sqrt{(k-1)^2 + k^2}}.$$

Finally, we show in Section 4 how the subset of the lattice points in  $[-k, k]^{d^2}$  over which the minimization is performed can be reduced, and discuss the computational efficiency of the resulting strategy. This makes it possible to determine values of  $\varepsilon(d, k)$  whose computation was previously intractable. Using this strategy, we compute  $\varepsilon(3, k)$  when  $4 \le k \le 8$ ,  $\varepsilon(4, k)$  when  $2 \le k \le 3$ , and  $\varepsilon(6, 1)$ . These values of  $\varepsilon(d, k)$  are the inverse of the numbers shown in bold in



Table 1. In addition, for each of the obtained values of  $\varepsilon(d, k)$ , we provide an explicit pair of lattice (d, k)-polytopes whose distance is precisely  $\varepsilon(d, k)$ . We shall refer to such a pair of polytopes as *kissing polytopes*.

#### 2. A least squares model for polytope distance

Let us consider two disjoint lattice (d, k)-simplices P and Q whose affine hulls are disjoint. Denote by  $p^0$  to  $p^n$  the vertices of P and by  $q^0$  to  $q^m$  the vertices of Q where n and m denote the dimension of P and Q, respectively. The distance of P and Q is the smallest possible value of

(1) 
$$\left\|\sum_{i=0}^{n}\lambda_{i}p^{i}-\sum_{i=0}^{m}\mu_{i}q^{i}\right\|^{2}$$

where  $\lambda_0$  to  $\lambda_n$  and  $\mu_0$  to  $\mu_m$  are two sets of non-negative numbers that each sum to 1. The constraint that each of these sets of numbers sum to 1 can be replaced by expressing  $\lambda_0$  and  $\mu_0$  as

(2) 
$$\begin{cases} \lambda_0 = 1 - \sum_{i=1}^n \lambda_i \\ \mu_0 = 1 - \sum_{i=1}^m \mu_i \end{cases}$$

and substituting them in (1) by these expressions. As a consequence,

$$d(P,Q)^{2} = \min_{\substack{\lambda \in \Delta_{n} \\ \mu \in \Delta_{m}}} f_{P,Q}(\lambda,\mu)$$

where

(3) 
$$f_{P,Q}(\lambda,\mu) = \left\| p^0 - q^0 + \sum_{i=1}^n \lambda_i (p^i - p^0) - \sum_{i=1}^m \mu_i (q^i - q^0) \right\|^2$$

and  $\Delta_j$  denotes the *j*-dimensional simplex

$$\Delta_j = \bigg\{ x \in [0, +\infty[^j] \colon \sum_{i=1}^j x_i \le 1 \bigg\}.$$

We will consider  $f_{P,Q}$  as a function from  $\mathbb{R}^n \times \mathbb{R}^m$  to  $[0, +\infty[$ . Note that this function depends on the ordering of the vertices of P and Q but this ordering will not play a role in the sequel, and we assume that a prescribed ordering has been fixed for the vertices of each pair of polytopes P and Q.

Relaxing the constraint that  $\lambda$  and  $\mu$  should be contained in  $\Delta_n$  and  $\Delta_m$  provides a lower bound on d(P,Q) of the form

(4) 
$$d(P,Q)^2 \ge \min_{\substack{\lambda \in \mathbb{R}^n \\ \mu \in \mathbb{R}^m}} f_{P,Q}(\lambda,\mu).$$

Note that the right-hand side of (4) is the distance between the affine hull of P and the affine hull of Q. In particular, the accuracy of this bound is related to how close the distance of P and Q is to the distance of their affine hulls.

Now consider the  $d \times (d-1)$  matrix

(5) 
$$A = \begin{bmatrix} p_1^1 - p_1^0 & \cdots & p_1^n - p_1^0 & q_1^1 - q_1^0 & \cdots & q_1^m - q_1^0 \\ \vdots & \vdots & \vdots & \vdots \\ p_d^1 - p_d^0 & \cdots & p_d^n - p_d^0 & q_d^1 - q_d^0 & \cdots & q_d^m - q_d^0 \end{bmatrix}$$

and the vector

$$b = q^0 - p^0$$

It will be important to keep in mind that A and b depend on P and Q. Observe that, with these notations, (3) can be rewritten into

(7) 
$$f_{P,Q}(\lambda,\mu) = \|A\chi - b\|^2$$

where  $\chi$  is the vector such that

(8) 
$$\chi^t = [\lambda_1, \cdots, \lambda_n, -\mu_1, \cdots, -\mu_m].$$

Remark 2.1: According to (7),  $f_{P,Q}(\lambda,\mu)$  is the sum of the squares of the coordinates of  $A\chi - b$ . In particular, negating both a row of A and the corresponding coefficient of b will not change the value of that function either. Likewise, negating a column of A and the corresponding row of  $\chi$  will not change the value of  $f_{P,Q}(\lambda,\mu)$ . As a consequence, the right-hand side of (4) does not change when a subset of the columns of A are negated or a subset of its rows are negated together with the corresponding coefficients of b.

Let us now give an expression for the right-hand side of (4).

LEMMA 2.2:  $f_{P,Q}$  admits a unique minimum over  $\mathbb{R}^n \times \mathbb{R}^m$  if and only if  $A^t A$  is non-singular. Moreover, in that case,

(9) 
$$\min_{\substack{\lambda \in \mathbb{R}^n \\ \mu \in \mathbb{R}^m}} f_{P,Q}(\lambda,\mu) = \left\| A(A^t A)^{-1} A^t b - b \right\|^2.$$

*Proof.* The minimum of  $f_{P,Q}$  is reached at a pair  $(\lambda, \mu)$  from  $\mathbb{R}^n \times \mathbb{R}^m$  such that all the partial derivatives of  $f_{P,Q}$  simultaneously vanish, that is when

$$\frac{\partial f_{P,Q}}{\partial \lambda_i}(\lambda,\mu) = 0$$

for all *i* satisfying  $1 \le i \le n$  and

$$\frac{\partial f_{P,Q}}{\partial \mu_i}(\lambda,\mu) = 0$$

for all *i* satisfying  $1 \leq i \leq m$ . Since  $f_{P,Q}$  is a quadratic function of  $\lambda$  and  $\mu$ , its partial derivatives are linear. In other words, finding the minimum of  $f_{P,Q}$ over  $\mathbb{R}^n \times \mathbb{R}^m$  amounts to solve a least squares problem. In particular setting to 0 all of these partial derivatives results in the system of linear equalities

(10) 
$$A^t A \chi = A^t b.$$

Since  $f_{P,Q}$  is a convex quadratic function, the solutions of (10) correspond bijectively via (8) with the pairs  $(\lambda, \mu)$  such that  $f_{P,Q}$  is minimal. It immediately follows that  $f_{P,Q}$  admits a unique minimum over  $\mathbb{R}^n \times \mathbb{R}^m$  if and only if  $A^t A$  is non-singular. Moreover, in that case, the unique solution of (10) is

$$\chi = (A^t A)^{-1} A^t b$$

and substituting this expression of  $\chi$  in (7) completes the proof.

According to (4), Lemma 2.2 provides a lower bound on d(P,Q) in the case when  $A^tA$  is non-singular. The following remark provides a necessary and sufficient condition on  $(A^tA)^{-1}A^tb$  for this bound to be sharp.

Remark 2.3: Recall that the minimum of  $f_{P,Q}$  over  $\mathbb{R}^n \times \mathbb{R}^m$  is the distance between the affine hulls of P and Q. Therefore, if  $A^t A$  is non-singular, then according to (7), (8), and Lemma 2.2, the first n coordinates of

$$\chi = (A^t A)^{-1} A^t b$$

provide an affine combination  $p^*$  of the vertices of P and its last m coordinates an affine combination  $q^*$  of the vertices of Q such that

$$d(p^{\star}, q^{\star}) = d(\operatorname{aff}(P), \operatorname{aff}(Q)).$$

In particular, if the first n coefficients of  $\chi$  are all non-negative and sum to at most 1 while its last m coefficients are all non-positive and sum to at least -1, then  $p^*$  belongs to P and  $q^*$  to Q. In that case, the distance of P and Qcoincides with the distance of their affine hulls. Otherwise the distance of Pand Q is strictly greater than the distance of their affine hulls.

We shall now focus on certain pairs of simplices whose distance is precisely  $\varepsilon(d, k)$ . The following is proven in [5] (see Theorem 5.2 therein).

THEOREM 2.4: There exist two lattice (d, k)-polytopes P and Q such that

- (i) d(P,Q) is equal to  $\varepsilon(d,k)$ ,
- (ii) both P and Q are simplices,
- (iii)  $\dim(P) + \dim(Q)$  is equal to d 1, and
- (iv) the affine hulls of P and Q are disjoint.

We shall prove that when P and Q satisfy the assertions (i) to (iv) in the statement of Theorem 2.4,  $f_{P,Q}$  admits a unique minimum over  $\mathbb{R}^n \times \mathbb{R}^m$  as a consequence of two results from [5]. The first of these results states that

(11) 
$$d(P,Q) \ge \varepsilon \left(\dim(P \cup Q), k\right)$$

(see Lemma 4.3 in [5]) and the second that, when k is fixed,  $\varepsilon(d, k)$  is a strictly decreasing function of d (see Theorem 5.1 in [5]).

PROPOSITION 2.5: If P and Q satisfy the assertions (i) to (iv) in the statement of Theorem 2.4, then  $f_{P,Q}$  has a unique minimum over  $\mathbb{R}^n \times \mathbb{R}^m$ . *Proof.* Denote by  $\operatorname{aff}(P)$  and  $\operatorname{aff}(Q)$  the affine hulls of P and Q, respectively. Consider a point  $p^*$  in  $\operatorname{aff}(P)$  and a point  $q^*$  in  $\operatorname{aff}(Q)$  such that

(12) 
$$\left\|q^{\star} - p^{\star}\right\| = d\left(\operatorname{aff}(P), \operatorname{aff}(Q)\right).$$

By the above discussion, the pair  $(p^*, q^*)$  corresponds to a point  $(\lambda^*, \mu^*)$ in  $\mathbb{R}^n \times \mathbb{R}^m$  where  $f_{P,Q}$  reaches its minimum. Assume that  $f_{P,Q}$  also reaches its minimum at a point  $(\overline{\lambda}^*, \overline{\mu}^*)$  in  $\mathbb{R}^n \times \mathbb{R}^m$  different from  $(\lambda^*, \mu^*)$ . By construction,  $(\overline{\lambda}^*, \overline{\mu}^*)$  then provides the coefficients of an affine combination  $\overline{p}^*$  of  $p^0$  to  $p^n$ and of an affine combination  $\overline{q}^*$  of  $q^0$  to  $q^m$  such that

(13) 
$$\left\|\overline{q}^{\star} - \overline{p}^{\star}\right\| = d\left(\operatorname{aff}(P), \operatorname{aff}(Q)\right).$$

Since  $p^*$  and  $\overline{p}^*$  are both contained in aff(P), so is their midpoint. Likewise, the midpoint of  $q^*$  and  $\overline{q}^*$  is contained in aff(Q). Hence,

(14) 
$$d(\operatorname{aff}(P), \operatorname{aff}(Q)) \leq \left\| \frac{q^{\star} + \overline{q}^{\star}}{2} - \frac{p^{\star} + \overline{p}^{\star}}{2} \right\|.$$

However, by the triangle inequality,

(15) 
$$\left\|\frac{q^{\star} + \overline{q}^{\star}}{2} - \frac{p^{\star} + \overline{p}^{\star}}{2}\right\| \leq \frac{1}{2} \left\|q^{\star} - p^{\star}\right\| + \frac{1}{2} \left\|\overline{q}^{\star} - \overline{p}^{\star}\right\|$$

with equality if and only if  $q^{\star} - p^{\star}$  is a multiple of  $\overline{q}^{\star} - \overline{p}^{\star}$  by a positive coefficient or one of these vectors is equal to 0. Under the assumption that assertion (iv) from the statement of Theorem 2.4 holds, these vectors are both non-zero. Hence,  $q^{\star} - p^{\star}$  is a multiple of  $\overline{q}^{\star} - \overline{p}^{\star}$  by a positive coefficient and according to (12) and (13), these vectors must therefore be equal. It immediately follows that the vectors  $\overline{p}^{\star} - p^{\star}$  and  $\overline{q}^{\star} - q^{\star}$  also coincide.

Now recall that  $(\lambda^*, \mu^*)$  and  $(\overline{\lambda}^*, \overline{\mu}^*)$  are different. As a consequence, so are the pairs  $(p^*, q^*)$  and  $(\overline{p}^*, \overline{q}^*)$ . Since the vectors  $\overline{p}^* - p^*$  and  $\overline{q}^* - q^*$  coincide they must therefore be non-zero. Hence, the translates of aff(P) and of aff(Q)through the origin of  $\mathbb{R}^d$  intersect in a non-zero vector and the dimension of their union must be less than dim(P) + dim(Q). As a consequence

$$\dim(P \cup Q) \le \dim(P) + \dim(Q).$$

Therefore, under the assumption that P and Q satisfy the assertion (iii) in the statement of Theorem 2.4, it follows that  $P \cup Q$  has dimension at most d-1. According to (11), this implies that the distance between P and Q is at least  $\varepsilon(d-1,k)$ . As a consequence, if the assertion (i) in the statement of Theorem 2.4 holds for P and Q, then one obtains that

$$\varepsilon(d,k) \ge \varepsilon(d-1,k).$$

However, Theorem 5.1 in [5] states that  $\varepsilon(d,k) < \varepsilon(d-1,k)$ . By this contradiction,  $f_{P,Q}$  has a unique minimum over  $\mathbb{R}^n \times \mathbb{R}^m$ .

Combining Proposition 2.5, Lemma 2.2, and Theorem 2.4, one obtains a lower bound on  $\varepsilon(d, k)$  from (4) of the form

(16) 
$$\varepsilon(d,k) \ge \min_{P,Q} \left\{ \left\| A(A^t A)^{-1} A^t b - b \right\| \right\}$$

where the minimum ranges over the pairs of lattice (d, k)-simplices P and Qwhose dimensions sum to d-1, for which the matrix A obtained from (5) is such that  $A^t A$  is non-singular and the vector b obtained from (6) satisfies

$$A(A^tA)^{-1}A^tb \neq b.$$

#### 3. The 2-dimensional case

In this section, we give a formula for  $\varepsilon(2, k)$  using the model described in Section 1. Consider two disjoint lattice (2, k)-polytopes P and Q that satisfy assertions (i) to (iv) from the statement of Theorem 2.4. Since the dimensions of P and Q sum to 1, one of these polytopes has dimension 0 and the other has dimension 1. We assume without loss of generality that P is a line segment and that Q is made of a single point by exchanging them if needed.

Let us first observe that according to (5) and (6),

$$\begin{cases} A = p^1 - p^0, \\ b = q^0 - p^0. \end{cases}$$

As a consequence, (16) simplifies into

$$\varepsilon(2,k) \geq \frac{|(p_2^1 - p_2^0)(q_1^0 - p_1^0) - (p_1^1 - p_1^0)(q_2^0 - p_2^0)|}{\sqrt{(p_1^1 - p_1^0)^2 + (p_2^1 - p_2^0)^2}}$$

It follows that  $\varepsilon(2, k)$  is at least the smallest possible value of

(17) 
$$\frac{|x_2x_3 - x_1x_4|}{\sqrt{x_1^2 + x_2^2}}$$

over all the lattice points x contained in the hypercube  $[-k, k]^4$  such that neither  $x_1^2 + x_2^2$  nor  $x_2x_3 - x_1x_4$  is equal to 0. We bound (17) as follows.

LEMMA 3.1: If k is greater than 1 then, for every lattice point x in  $[-k, k]^4$  such that  $x_1^2 + x_2^2$  and  $x_2x_3 - x_1x_4$  are both non-zero,

(18) 
$$\frac{|x_2x_3 - x_1x_4|}{\sqrt{x_1^2 + x_2^2}} \ge \frac{1}{\sqrt{(k-1)^2 + k^2}}.$$

Proof. Consider a lattice point x in  $[-k, k]^4$  such that neither  $x_1^2 + x_2^2$  nor  $x_2x_3 - x_1x_4$  is equal to 0. We assume without loss of generality that  $x_1$  and  $x_2$  are non-negative thanks to the symmetries of  $[-k, k]^4$ . We review two cases.

First assume that  $x_1$  and  $x_2$  coincide. In that case,

(19) 
$$\frac{|x_2x_3 - x_1x_4|}{\sqrt{x_1^2 + x_2^2}} = \frac{|x_3 - x_4|}{\sqrt{2}}$$

Since  $x_2x_3 - x_1x_4$  is not equal to 0,  $x_3$  and  $x_4$  cannot coincide and the righthand side of (19) is at least  $1/\sqrt{2}$ . As k is greater than 1,

$$\frac{1}{\sqrt{(k-1)^2 + k^2}} \le \frac{1}{\sqrt{2}}$$

and the lemma follows in this case.

Now assume that  $x_1$  and  $x_2$  are different. Since  $|x_2x_3 - x_1x_4|$  is at least 1,

(20) 
$$\frac{|x_2x_3 - x_1x_4|}{\sqrt{x_1^2 + x_2^2}} \ge \frac{1}{\sqrt{x_1^2 + x_2^2}}$$

Recall that  $x_1$  and  $x_2$  are integers contained in [0, k]. Since they are different, one of them is at most k - 1. As a consequence,

$$\frac{1}{\sqrt{x_1^2 + x_2^2}} \ge \frac{1}{\sqrt{(k-1)^2 + k^2}}$$

and combining this with (20) completes the proof.

By Lemma 3.1, and the preceding discussion,  $\varepsilon(2, k)$  is at least the right-hand side of (18) when k is at least 2. Theorem 1.1 states that this is sharp.

Proof of Theorem 1.1. It suffices to exhibit a lattice point P and a lattice segment Q contained in the square  $[0, k]^2$  such that

$$d(P,Q) = \frac{1}{\sqrt{(k-1)^2 + k^2}}.$$

Such an example is provided by the point in  $[0, k]^2$  whose two coordinates are equal to 1 and any of the two line segments that are incident to the origin



Figure 1. A pair of kissing lattice (2, 4)-polytopes.

and whose other vertex has coordinates k and k-1. This point and this line segment are represented in Figure 1 when k is equal to 4.

Remark 3.2: The strategy exposed in this section in the 2-dimensional case can be generalized to any higher dimension. In particular, a quotient similar to (17) can be explicitly computed in any fixed dimension d that depends on a lattice point x contained in the hypercube  $[-k, k]^{d^2}$ . The first d(d-1) coordinates of x are the entries of A and its last d coordinates are the coordinates of b. The minimum of that quotient under the constraint that its numerator and denominator are positive provides a lower bound on  $\varepsilon(d, k)$ . For instance, when d is equal to 3, the minimal value of the ratio

(21) 
$$\frac{|x_1(x_6x_8 - x_5x_9) + x_2(x_4x_9 - x_6x_7) + x_3(x_5x_7 - x_4x_8)|}{\sqrt{(x_1x_5 - x_2x_4)^2 + (x_1x_6 - x_3x_4)^2 + (x_2x_6 - x_3x_5)^2}}$$

over all the lattice points x in  $[-k, k]^9$  such that the numerator and the denominator of (21) are positive is a lower bound on  $\varepsilon(3, k)$ . However, the expression for this quotient gets complicated as the dimension increases and solving the corresponding integer minimization problem becomes involved.

#### 4. The computation of $\varepsilon(d, k)$

According to the discussion in Section 1, a lower bound on  $\varepsilon(d, k)$  can be obtained by considering all the sets of d+1 pairwise distinct points from  $\{0, \ldots, k\}^d$  and for each such set  $\mathcal{S}$ , all the partitions of  $\mathcal{S}$  into two subsets  $\{p^0, \ldots, p^n\}$  and  $\{q^0, \ldots, q^m\}$  where n + m is equal to d - 1. For each such partition, one can

build a matrix A and a vector b according to (5) and (6). The smallest possible non-zero value of the right-hand side of (16) over all the obtained pairs (A, b)such that  $A^t A$  is non-singular will then be a lower bound on  $\varepsilon(d, k)$ . However, this strategy requires to consider

$$N = (2^{d+1} - 2) \binom{(k+1)^d}{d+1}$$

pairs (A, b). Note that while this number would decrease to at best

$$\frac{2^{d+1}-2}{2^d d!} \binom{(k+1)^d}{d+1}$$

if the enumeration could be performed up to the symmetries of the *d*-dimensional hypercube. However, these symmetries are not all easy to handle in practice as one still needs to enumerate all N pairs (A, b) just to check for them.

We adopt a different strategy in order to significantly decrease the search space without having to handle symmetries. The main idea is to do the enumeration coordinate-wise in order to build a list  $\mathcal{L}$  of the possible rows for the pair (A, b) for each n and m that sum to d - 1 and such that  $n \leq m$ , and then building (A, b) back by selecting d pairwise different rows from  $\mathcal{L}$ . By a row of (A, b), we mean a vector r from  $\mathbb{R}^d$  whose first d - 1 entries form a row of A and whose last entry is the corresponding coordinate of b. Note that our requirement that the rows of  $\mathcal{L}$  selected to build a given pair (A, b) are pairwise distinct is without loss of generality. Indeed, if two of these rows would coincide, a pair of columns of  $A^t A$  would be multiples of one another and that matrix would then be singular. We shall see that the size of  $\mathcal{L}$  does not depend on nor m. As a consequence, this alternative strategy only considers

$$\left\lfloor \frac{d+1}{2} \right\rfloor \binom{|\mathcal{L}|}{d}$$

pairs (A, b). For each of these pairs such that  $A^t A$  is non-singular, the righthand side of (16) is evaluated, and the smallest non-zero value obtained for this quantity over all the considered pairs (A, b) is the desired lower bound on  $\varepsilon(d, k)$ . Note that the efficiency of this strategy depends on how large  $\mathcal{L}$  is. Let us get into more details about how we build  $\mathcal{L}$ .

For a given pair of positive integers n and m that sum to d-1, we generate all the possible rows of the pair (A, b) as

(22) 
$$(x_1 - x_0, \dots, x_n - x_0, y_1 - y_0, \dots, y_m - y_0, y_0 - x_0)$$

where x is a point from  $\{0, \ldots, k\}^n$ , y is a point from  $\{0, \ldots, k\}^m$  such that x and y are not both equal to 0, and  $x_0$  and  $y_0$  are two integers from  $\{0, \ldots, k\}$ . The list obtained from this procedure contains at most  $(k-1)^{d+1}$  rows. It can be reduced using the following property.

PROPOSITION 4.1: Consider a  $d \times (d-1)$  matrix A with integer entries such that  $A^t A$  is non-singular and a vector b from  $\mathbb{Z}^d$ . If the pair  $(\overline{A}, \overline{b})$  is obtained by dividing each row of the pair (A, b) by the greatest common divisor of its coordinates and by negating a subset of the resulting rows, then

(23) 
$$\left\| A(A^{t}A)^{-1}A^{t}b - b \right\| \ge \left\| \overline{A}(\overline{A}^{t}\overline{A})^{-1}\overline{A}^{t}\overline{b} - \overline{b} \right\|$$

and the two sides of this inequality are either both zero or both positive.

*Proof.* Pick two non-negative integers n and m that sum to d-1. Denote b by  $q^0$ . Likewise, denote by  $p^1$  to  $p^n$  the first n columns of A and consider the points  $q^1$  to  $q^m$  from  $\mathbb{Z}^d$  such that  $q^1 - q^0$  to  $q^m - q^0$  are the last m columns of A. According to the construction described in Section 1,

(24) 
$$\left\|A(A^{t}A)^{-1}A^{t}b - b\right\|^{2} = \min_{\substack{\lambda \in \mathbb{R}^{n} \\ \mu \in \mathbb{R}^{m}}} f_{P,Q}(\lambda,\mu)$$

where P is the convex hull of  $p^0$  to  $p^n$  and Q that of  $q^0$  to  $q^m$ . Further denote by  $(\overline{A}, \overline{b})$  the pair obtained by dividing each row of (A, b) by the greatest common divisor of its coordinates and by negating a fixed (but otherwise arbitrary) subset of the resulting rows. As above,

(25) 
$$\left\|\overline{A}(\overline{A}^{t}\overline{A})^{-1}\overline{A}^{t}\overline{b} - \overline{b}\right\|^{2} = \min_{\substack{\lambda \in \mathbb{R}^{n} \\ \mu \in \mathbb{R}^{m}}} f_{\overline{P},\overline{Q}}(\lambda,\mu)$$

where  $\overline{P}$  and  $\overline{Q}$  are the convex hulls of the points  $\overline{p}^0$  to  $\overline{p}^n$  and  $\overline{q}^0$  to  $\overline{q}^m$  that are extracted from  $(\overline{A}, \overline{b})$  just as the points  $p^i$  and  $q^i$  are extracted from (A, b). By construction, for any pair  $(\lambda, \mu)$  of vectors in  $\mathbb{R}^n \times \mathbb{R}^m$ ,

(26) 
$$\sum_{j=1}^{d} \left( -q_j^0 + \sum_{i=1}^{n} \lambda_i p_j^i - \sum_{i=1}^{m} \mu_i (q_j^i - q_j^0) \right)^2 = \sum_{j=1}^{d} r_j^2 \left( -\overline{q}_j^0 + \sum_{i=1}^{n} \lambda_i \overline{p}_j^i - \sum_{i=1}^{m} \mu_i (\overline{q}_j^i - \overline{q}_j^0) \right)^2$$

where  $r_1$  to  $r_d$  the greatest common divisors of the rows of (A, b). Observe that according to (3), the right-hand side of this equality is precisely  $f_{P,Q}(\lambda, \mu)$ . Since the numbers  $r_1$  to  $r_d$  are not less than 1, its right-hand side is at least  $f_{\overline{P},\overline{O}}(\lambda,\mu)$  and it follows that, for every  $(\lambda,\mu)$  in  $\mathbb{R}^n \times \mathbb{R}^m$ ,

$$f_{P,Q}(\lambda,\mu) \ge f_{\overline{P},\overline{Q}}(\lambda,\mu)$$

In turn, by (24) and (25), the desired inequality holds. It remains to show that if the right-hand side of (23) is equal to 0, then so is its left-hand side.

Assume that the right-hand side of (23) is equal to 0. In that case, there exists a pair  $(\lambda, \mu)$  of vectors in  $\mathbb{R}^n \times \mathbb{R}^m$  such that  $f_{\overline{P},\overline{Q}}(\lambda,\mu)$  is equal to 0. According to (3),  $f_{\overline{P},\overline{Q}}(\lambda,\mu)$  is the squared norm of a vector and since it is equal to 0, all of the coordinates of that vector must be equal to 0. In other words, for every integer j satisfying  $1 \le j \le d$ ,

$$-\overline{q}_j^0 + \sum_{i=1}^n \lambda_i \overline{p}_j^i - \sum_{i=1}^m \mu_i \left(\overline{q}_j^i - \overline{q}_j^0\right) = 0$$

and it follows from (3) and (26) that  $f_{P,Q}(\lambda, \mu)$  must vanish. According to (24), the left-hand side of (23) is then equal to 0, as desired.

By Proposition 4.1, we can assume that when several of the generated rows are multiples of one another, only the one among them whose coordinates are relatively prime and whose first non-zero coordinate is positive is included in  $\mathcal{L}$ . It should be observed that, before  $\mathcal{L}$  is reduced as we have just described, its size does not depend on n or m. As announced, this property still holds once  $\mathcal{L}$  has been reduced. Indeed, observe that the rows generated by (22) with the same two points x and y and the same scalars  $x_0$  and  $y_0$  but with different values of n and m can be recovered from one another by adding  $y_0 - x_0$  to (or

d	k									
	1	2	3	4	5	6	7	8	9	10
3	6	24	72	144	288	432	720	1008	1440	1872
4	14	89	359	929	2189	4019	7469	11969		
5	30	300	1620	5400	15120					
6	62	965	6971							
7	126	3024								

Table 2. The number of rows in  $\mathcal{L}$  as a function of d and k.

subtracting this quantity from) certain of their coordinates. Hence, all of these rows have the same greatest common divisor for their coordinates.

We report in Table 2 as a function of d and k the number of rows contained in  $\mathcal{L}$  after this procedure has been carried out. Note that, when k is equal to 1, d to 3, n to 1, and m to 1, there are only 6 rows in  $\mathcal{L}$ :

$$\mathcal{L} = \left\{ (1,0,0), (0,1,0), (1,-1,0), (0,1,-1), (1,1,-1), (1,0,-1) \right\}.$$

Twenty pairs (A, b) are generated from this list of rows. When k is equal to 3 and d to 4, the number of pairs (A, b) that have to be considered with the approach outlined at the beginning of the section is

$$(2^5 - 2)\binom{4^4}{5} = 264\,286\,471\,680$$

which would shrink down to

$$\frac{2^5 - 2}{2^4 4!} \binom{4^4}{5} = 688\,246\,020$$

if these pairs could be enumerated up to the symmetries of the hypercube. However, there is no easy way to test for these symmetries without reviewing all of the 264 286 471 680 pairs. With our approach,  $|\mathcal{L}|$  is equal to 359 in that case as shown in Table 2 and we only need to consider

$$2\binom{359}{4} = 1\,361\,176\,502$$

pairs (A, b) in order to compute our lower bound on  $\varepsilon(4, 3)$ .

This strategy does not only provide a lower bound on  $\varepsilon(d, k)$  but also pairs (A, b) that achieve this lower bound. Keeping track of the points x and y and of the scalars  $x_0$  and  $y_0$  that are used to build each row in  $\mathcal{L}$  according to (22), one can recover two lattice (d, k)-polytopes P and Q such that the obtained lower bound on  $\varepsilon(d, k)$  is precisely the distance of the affine hulls of P and Q. If the distance between these affine hulls coincides with the distance between P and Q, which can easily be checked from the pair (A, b) according to Remark 2.3, then this lower bound is sharp. Interestingly, using this observation, all the lower bounds on  $\varepsilon(d, k)$  that we have obtained using the presented computational strategy have turned out to be the precise value of  $\varepsilon(d, k)$ .

The known values of  $\varepsilon(d, k)$  are reported in Table 1 in the case when d is at least 3. Recall that  $\varepsilon(2, k)$  is given by Theorem 1.1 for all k greater than 1. Moreover,  $\varepsilon(2, 1)$  is equal to  $1/\sqrt{2}$ . The values shown in bold characters in



Figure 2. A pair of kissing lattice (3, 4)-polytopes.

the table are the ones that were obtained using the strategy described in this section. The other values of  $\varepsilon(d, k)$  given in the table were previously obtained in [5]. Let us now describe the polytopes P and Q that have been obtained in each case whose distance is precisely  $\varepsilon(d, k)$ .

If k is equal to 2, 4, 5, 6, 7, or 8, then  $\varepsilon(3, k)$  is achieved by the line segment P with vertices (0, 0, 0) and (k - 1, k, k) and the line segment Q with vertices (k, 1, 2) and (0, k, k - 1). These two line segments are shown in Figure 2 when k is equal to 4. Note that in general, their distance is

(27) 
$$d(P,Q) = \frac{1}{\sqrt{2(2k^2 - 4k + 5)(2k^2 - 2k + 1)}}$$

and it is tempting to ask whether  $\varepsilon(3, k)$  is equal to this value for every integer k greater than 8. In any case, note that the right-hand side of (27) provides an upper bound on  $\varepsilon(3, k)$  that decreases like  $1/(2\sqrt{2}k^2)$  as k goes to infinity. In the remaining two cases, when k is equal to either 1 or 3, the line segments that achieve  $\varepsilon(3, k)$  do not follow the pattern we have just described. Indeed,  $\varepsilon(3, 1)$  is the distance between a diagonal P of the cube  $[0, 1]^3$  and a diagonal Q of one of its square faces such that P and Q are disjoint (see also [5]) while  $\varepsilon(3, 3)$  is the distance between the line segment with vertices (0, 0, 0) and (2, 3, 3) and the line segment with vertices (3, 2, 0) and (0, 1, 2).

In the 4-dimensional case, the values of  $\varepsilon(4, k)$  reported in Table 1 are always achieved by a line segment P and a triangle Q as follows. When k is equal to 1, the vertices of P are (0,0,0,0) and (1,1,1,1) while the vertices of Q are (1,0,0,0), (0,1,1,0), and (0,1,0,1). When k is greater than 1, the vertices of P are (0,0,0,0) and (1,2,1,2) and those of Q are (2,2,1,0), (0,1,0,2), and (0,0,2,1). When k is equal to 3, the vertices of P are (0,0,1,0) and (2,3,3,3) and the vertices of Q are (3,0,3,2), (0,2,0,3), and (0,3,3,0).

The unique value of  $\varepsilon(5, k)$  reported in Table 1 is the one when k is equal to 1. This value is the distance between the diagonal of the hypercube  $[0,1]^5$ incident to the origin of  $\mathbb{R}^5$  and the tetrahedron with vertices (1,1,0,0,0), (0,1,0,1,1), (0,0,1,0,1), and (0,0,1,1,0). Finally,  $\varepsilon(6,k)$  is equal to the distance between the diagonal of the hypercube  $[0,1]^6$  incident to the origin of  $\mathbb{R}^6$  and the 5-dimensional simplex with vertices (1,0,1,1,0,0), (1,0,0,0,1,1), (0,1,1,0,1,1), (0,1,0,1,0,1), and (0,1,0,1,1,0).

Remark 4.2: It is noteworthy that, while  $\varepsilon(2, k)$  can be guessed from the pairs of kissing polytopes obtained for the first few values of k, this is not the case for  $\varepsilon(d, k)$  when k is fixed. Even when k is equal to 1, the pairs of kissing polytopes known for the first few values of d do not exhibit a clear pattern.

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