ON THE BOUNDEDNESS OF AN ITERATION INVOLVING
POINTS ON THE HYPERSPHERE

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Abstract. For a finite set of points $X$ on the unit hypersphere in $\mathbb{R}^d$ we consider the iteration $u_{i+1} = u_i + \chi_i$, where $\chi_i$ is the point of $X$ farthest from $u_i$. Restricting to the case where the origin is contained in the convex hull of $X$ we study the maximal length of $u_i$. We give sharp upper bounds for the length of $u_i$ independently of $X$. Precisely, this upper bound is infinity for $d \geq 3$ and $\sqrt{2}$ for $d = 2$.

1. Introduction and overview

Throughout this paper we will assume that $d \geq 2$. By $\mathbb{R}^d$ we denote $d$-dimensional Euclidean space, equipped with the standard scalar product $\langle \cdot, \cdot \rangle$ and induced norm $\| \cdot \|$. Moreover $S^l(r)$ denotes the $l$-dimensional sphere of radius $r$, and $S^l := S^l(1)$. These spheres are always considered as embedded in $\mathbb{R}^d$. Let $X = \{x_1, \ldots, x_n\} \subseteq S^{d-1} \subseteq \mathbb{R}^d$ be a finite set on the unit hypersphere. Without mentioning this each time, we assume that the linear space spanned by the elements of $X$ equals $\mathbb{R}^d$, i.e. $d$ cannot be reduced. Consider the iteration

$$u_0 := 0, \quad u_{i+1} := u_i + \chi_i,$$

where $i \in \mathbb{N}_0$ and $\chi_i$ is the element of $X$ which is farthest away from $u_i$ (which happens to be $\text{argmin}_{x \in X} \langle x, u_i \rangle$). In case there are several elements of $X$ at maximal distance, just choose any of them. Due to this ambiguity there are many iterations $(u_i)_{i=0}^\infty$ for a particular set $X$. By $U(X)$ we denote the set of vectors occurring in any of these iterations. Let

$$u^*(X) := \sup \{ \|u\| \mid u \in U(X) \}$$

be the greatest length reached during any of these iterations. The question which values $u^*(X)$ can take is simple and intriguing; it was brought up in connection with the rate of convergence of an iterative approach of computing the smallest enclosing ball of a point set, as described in the following.

Let $\tilde{Y} \subseteq \mathbb{R}^d$ be a finite set of points. Then the smallest enclosing ball $\text{SEB}(\tilde{Y})$ of $\tilde{Y}$ exists and is unique [Wel91]. We assume that $\tilde{Y}$ has at least two elements. By
\( c \in \mathbb{R}^d \) and \( R \in \mathbb{R}^+ \) we denote center and radius of \( \text{SEB}(\tilde{Y}) \), respectively. Bădoiu and Clarkson [BC03] introduced the following approximation of \( c \):

\[
c_0 := 0, \quad c_{i+1} := c_i + \frac{1}{i+1}(\xi_i - c_i), \tag{1}
\]

where \( i \in \mathbb{N} \) and \( \xi_i \) is the element of \( \tilde{Y} \) farthest away from \( c_i \). This approximation \((c_i)_{i=0}^\infty\) is related to the iteration \((u_i)_{i=0}^\infty\) by \( Ru_i = i(c_i - c) \) which implies \( u_{i+1} = u_i + \frac{\xi_i - c}{R} \). The set \( \tilde{X} \) connected to \((u_i)_{i=0}^\infty\) is given by

\[
\tilde{X} := \left\{ \frac{1}{R}(y - c) \mid y \in \tilde{Y} \right\}. \tag{2}
\]

Unlike \( X \) the set \( \tilde{X} \) can contain also points in the interior of the unit hypersphere. Martinetz, Madany and Mota [MMM06] show that after a finite number of steps all \( \xi_i \) will lie on the boundary of \( \text{SEB}(\tilde{Y}) \), i.e. \( \xi_i \in Y \) for all \( i \geq i_0 \), where \( Y \subseteq \tilde{Y} \) consists of all points on the surface of \( \text{SEB}(\tilde{Y}) \). This clarifies the correspondence.

While the approximation is extremely easy to use, the question of convergence needs to be answered. In [BC03] it is shown that for \( i \in \mathbb{N} \)

\[
\|c - c_i\| \leq \frac{1}{\sqrt{i}}. \tag{3}
\]

[MMM06] aims at proving faster convergence than (3). In particular:

**Theorem 1** ([MMM06], Theorem 2). Let \( \tilde{Y} \subseteq \mathbb{R}^d \) be a finite set with at least two elements, and let \( \tilde{X} \) be given by (2). Consider the approximation (1) of \( \text{SEB}(\tilde{Y}) \). Then for all \( i \in \mathbb{N} \)

\[
\|c - c_i\| \leq \frac{u^*(\tilde{X})}{i},
\]

where the definition of \( u^* \) has been extended to sets \( \tilde{X} \) with points on or in the interior of the unit hypersphere in a straightforward manner.

In view of Theorem 1 a finite value of \( u^* \) or even a uniform upper bound independent of \( X \) is desirable. Before stating our results on the latter, we need some preparations.

The connection between \((c_i)_{i=0}^\infty\) and \((u_i)_{i=0}^\infty\) is further illustrated by

**Proposition 2.** For a finite set \( X \subseteq S^{d-1} \subseteq \mathbb{R}^d \) the following statements are equivalent.

(i) \( \text{SEB}(X) = S^{d-1} \),

(ii) The origin \( 0 \in \mathbb{R}^d \) is contained in \( \text{conv}(X) \),

(iii) \( \delta(X) \geq 0 \), where

\[
\delta(X) := -\max_{\|u\|=1} \min_{x \in X} \langle x, u \rangle.
\]
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Proof. (i)$\iff$(ii) is due to R. Seidel (cf. Lemma 1 in [FGK03]). (ii)$\iff$(iii) follows from the fact that a point $p \in \mathbb{R}^d$ lies in the convex hull of $X$ if and only if $\min_{x \in X} \langle x - p, u \rangle \leq 0$ for all unit vectors $u$. □

$X$ is called 0-balanced if $0 \not\in \operatorname{conv}(X)$. For $1 \leq b \leq d - 1$ the set $X$ is called $b$-balanced, if 0 is on the boundary of $\operatorname{conv}(X)$ and is contained in a $b$-dimensional face, but not in a $(b - 1)$-dimensional face of $\operatorname{conv}(X)$. If 0 is an inner point of $\operatorname{conv}(X)$, then $X$ is called $d$-balanced or balanced. Having the same balance property is an equivalence relation on all sets $X$ under consideration.

Note that $\delta(X)$ is strictly positive if and only if $X$ is $d$-balanced, and Proposition 2 characterizes all sets $X$ that are not 0-balanced.

Theorem 3. Let $X$ be a finite set of unit vectors in $\mathbb{R}^d$.

(i) If $X$ is 0-balanced, then $u^*(X) = \infty$.
(ii) If $X$ is $b$-balanced for $0 < b \leq d$, then $u^*(X) < \infty$.

Proof. Again, (ii) is shown in [MMM06]; it remains to prove (i). Since $\operatorname{conv}(X)$ is compact, there is a point $T \in \operatorname{conv}(X)$ which is closest to the origin. Let $\epsilon := |OT|$. Clearly $||\chi_j|| \geq \epsilon$ for all $j \in \mathbb{N}_0$, therefore $||u_i|| = ||\sum_{j=0}^{i-1} \chi_j|| \geq i\epsilon$ is an unbounded sequence for $i \in \mathbb{N}_0$. □

For $0 \leq b \leq d$ we define

$$u_{d,b}^{**} := \sup \{ u^*(X) \mid X \subseteq S^{d-1} \subseteq \mathbb{R}^d \text{ finite and b-balanced} \}.$$

Our goal is to compute $u_{d,b}^{**}$ for all possible $d$ and $b$.

Theorem 4. For $d = 2$ we have $u_{2,0}^{**} = \infty$, while $u_{2,1}^{**} = u_{2,2}^{**} = \sqrt{2}$.

Clearly, for $d = 2$, $X = \{x_1, x_2\}$, $x_1 = (0, 1)$, $x_2 = (1, 0)$ the iteration $u_0 = 0$, $u_1 = x_1$, $u_2 = x_1 + x_2$ is valid and $||u_2|| = \sqrt{2}$. This manifest example represents one inequality of the proof of Theorem 4; the missing inequality is shown in Section 2.

Theorem 5. For $d \geq 3$ we have $u_{d,b}^{**} = \infty$ for all $0 \leq b \leq d$.

Proof. For any dimension $d$ we have $u_{d,0}^{**} = \infty$ from Theorem 3 (i). For $1 \leq b \leq d - 2$ the assertion follows from the example discussed in Proposition 13 below. For $b = d$ and $b = d - 1$ use Proposition 15 (ii) and (iii), respectively. □

Although the balance property of $X$ is a suggesting geometric property, it does not seem to give a finer prediction for $u^*(X)$ than $\delta(X)$. In the balanced case, $0 < \delta(X)$ determines a finite upper bound for $u^*(X)$ as shown in [MMM06], namely

$$||u_i|| \leq \frac{1}{2\delta(X)} + 1, \quad i \in \mathbb{N}_0.$$
With respect to the faster convergence we have an immediate result for \( d = 2 \):

**Corollary 6.** Let \( \tilde{Y} \subseteq \mathbb{R}^2 \) be a finite set with at least two elements. Assume that all elements of \( \tilde{Y} \) lie on the boundary of \( \text{SEB}(\tilde{Y}) \). Then \( \|c - c_i\| \leq \frac{\sqrt{2}R_i}{\pi} \) for all \( i \in \mathbb{N} \).

2. **Proof for** \( d = 2 \)

Let \( e_1, e_2 \) denote the canonical orthonormal basis of \( \mathbb{R}^2 \). Each \( x_j \in X \), \( 1 \leq j \leq n \) can be written as

\[
x_j = \cos(\phi_j) e_1 + \sin(\phi_j) e_2 = [1; \phi_j],
\]

where \([\tilde{r}; \tilde{\phi}]\) indicates a point in standard polar coordinates on \( \mathbb{R}^2 \). Similarly, for \( j \in \mathbb{N} \) we write

\[
\chi_j = \cos(\psi_j) e_1 + \sin(\psi_j) e_2 = [1; \psi_j],
\]

\[
u_j = \lambda_j \left( \cos(\alpha_j) e_1 + \sin(\alpha_j) e_2 \right) = [\lambda_j; \alpha_j],
\]

All argument angles are real numbers taken modulo \( 2\pi \). The freedom in rotation is fixed as follows. Assume that \( x_1, \ldots, x_n \) are numbered counterclockwise, starting at \( \phi_1 = 2\pi - \phi \), ending at \( \phi_n = \pi + \phi \), such that there is a gap with angle size \( \pi - 2\phi \) between the two neighboring elements \( x_1, x_n \) of \( X \) is symmetric about the \( e_2 \)-axis. We call this a parametrization of \( X \) with base gap of size \( \pi - 2\phi \), where \( \phi \in [0, \frac{\pi}{2}) \). The choice of \( \phi \) indicates that we restrict to the balanced cases.

Define \( \bar{\phi} := \frac{\pi}{6} - \phi \). For \( W \subseteq \mathbb{R}^2 \) and \( k = 1, \ldots, n \) let \( T_k(W) \) denote the set obtained by translation of \( W \) by \( x_k \). The set \( T \) is defined by

\[
T := \left\{ [\tilde{r}; \tilde{\phi}] \in \mathbb{R}^2 \mid \tilde{r} \in (1, \sqrt{2}] \text{ and } \tilde{\phi} \in \left( \frac{\pi}{2} - \bar{\phi}, \frac{\pi}{2} + \bar{\phi} \right) \right\}.
\]

Moreover, we define three subsets of \( \mathbb{R}^2 \) by

\[
R := \{ [\tilde{r}; \tilde{\phi}] \mid \tilde{r} > 0 \text{ and } \tilde{\phi} \in (\pi - \phi, 2\pi + \phi) \},
\]

\[
Q := \{ (a, b) \mid |a| \tan \phi \leq b \leq |a| \tan \phi + \lambda_{\min} \},
\]

\[
P := \{ u \in \mathbb{R}^2 \mid \|u\| \leq 1 \} \setminus (R \cup Q).
\]

Here \( \lambda_{\min} := \frac{\sqrt{3}}{2\cos \phi} \) is the length of the intersection of \( Q \) with the \( e_2 \)-axis. Figure[1] gives an illustration of this situation; [FIG] gives an animated version where \( \phi \) varies in time.

**Lemma 7.** Let \( X \) be a finite subset of \( S^1 \subseteq \mathbb{R}^2 \), parametrized as above. Suppose that \( \phi \in [0, \frac{\pi}{8}) \), i.e. the size of the base gap is greater than \( \frac{\pi}{8} \). Define the set \( V \) by

\[
V := P \cup T_n(P^+) \cup T_1(P^-) \cup Q \cup R,
\]

where \( P^+, P^- \) denote the elements of \( P \) with non-negative and non-positive \( e_1 \)-coordinate, respectively. Then \( u_j \in V \) for all \( j \in \mathbb{N}_0 \).
Figure 1. An arbitrary set $X \subseteq S^1 \subseteq \mathbb{R}^2$ given in base gap parametrization. Only $x_1$ and $x_n$ are displayed, the remaining elements of $X$ are above $x_1$ and $x_n$. Recall that $\phi + \bar{\phi} = \frac{\pi}{6}$. $R$ is the open set bounded from above by the lower dashed lines. $Q$ is the closed set between the dashed lines. The set $P$ is given by the central hatched area. For small values of $\phi$, $T_1(P^-) \setminus (Q \cup R)$ and $T_n(P^+) \setminus (Q \cup R)$ are nonempty.

Proof. Clearly $u_0 \in V$. By induction, assume that $u_j \in V$ for some $j \in \mathbb{N}$. The proof is complete if all of the following claims are shown to be true.

(a) If $u_j \in Q$, then $u_{j+1} \in Q \cup R$.
(b) If $u_j \in P$, then $u_{j+1} \in T_n(P^+) \cup T_1(P^-)$.
(c) If $u_j \in R$, then $u_{j+1} \in P \cup Q \cup R$.
(d) If $u_j \in T_n(P^+)$, then $u_{j+1} \in P \cup Q \cup R$.
(e) If $u_j \in T_1(P^-)$, then $u_{j+1} \in P \cup Q \cup R$.

If $u_j \in P \cup Q$, then $x_1$ or $x_n$ is chosen in the next step of the iteration, i.e. $\chi_j \in \{x_1, x_n\}$. Therefore, (b) is trivial. Also (a) is true since $T_1(Q)$ and $T_n(Q)$ have no parts above $Q$. If (d) is true then (e) holds by symmetry. Hence it suffices to show (c) and (d).
Claim (c). Suppose that \( u_j \in R \) is arbitrarily fixed. If \( \alpha_j \in (\pi + \phi, 2\pi - \phi) \), then from Figure 1 it is clear that translation of the part of \( R \) with such argument \( \alpha_j \) by an arbitrary unit vector stays inside \( P \cup Q \cup R \).

Otherwise, \( \alpha_j \in [\phi, \phi) \) or \( \alpha_j \in (\pi - \phi, \pi + \phi] \), where the second part follows from the first by symmetry. Restricting to \( \alpha := \alpha_j \in [\phi, \phi) \) and setting \( \lambda := \lambda_j > 0 \), \( \psi := \psi_j \in [\pi + 2\alpha - \phi, \pi + \phi] \) we can write

\[
 u_{j+1} = (\lambda \cos \alpha + \cos \psi)e_1 + (\lambda \sin \alpha + \sin \psi)e_2.
\]

The range of \( \psi \) follows since the center of the interval of possible values for \( \psi \) is \( \alpha + \pi \), it extends by \( \pi + \phi - (\alpha + \pi) = \phi - \alpha \) to both sides. We continue to work on two cases.

(c.i) The \( e_1 \)-coordinate of \( u_{j+1} \) is non-negative. In this case \( \sin(\psi - \phi) \leq \frac{\sqrt{3}}{2} \) and \( \lambda \sin(\phi - \alpha) \geq 0 \). Since equality does not hold simultaneously,

\[
0 < \lambda \sin(\phi - \alpha) + \sin(\phi - \psi) + \frac{\sqrt{3}}{2}.
\]

Expanding and rearranging the trigonometric terms, substituting \( \lambda_{\text{min}} = \frac{\sqrt{3}}{2 \cos \phi} \) (which denotes the length of the intersection of \( Q \) with the \( e_2 \)-axis) and dividing by \( \cos \phi > 0 \) we get

\[
(\lambda \sin \alpha + \sin \psi) - \lambda_{\text{min}} < \tan \phi (\lambda \cos \alpha + \cos \psi).
\]

This shows that \( u_{j+1} \) falls below the line bounding \( Q \) from above. Hence \( u_{j+1} \in Q \cup R \).

(c.ii) The \( e_1 \)-coordinate of \( u_{j+1} \) is negative, i.e. \( \lambda < -\frac{\cos \psi}{\cos \alpha} \). If we knew the inequality

\[
\frac{\cos \psi}{\cos \alpha} \geq 2 \cos(\psi - \alpha), \tag{4}
\]

then \( \lambda \leq -2 \cos(\psi - \alpha) \) would follow using the inequality for \( \lambda \). We would arrive at

\[
\|u_{j+1}\|^2 = 1 + \lambda^2 + 2\lambda \cos(\psi - \alpha) \leq 1,
\]

which would show that \( u_{j+1} \in P \cup Q \cup R \). Hence we are left with (4).

First consider the case \( \alpha \geq 0 \). Then \( 2 \cos(\psi - \alpha) < -\sqrt{3} \) and

\[
\frac{\cos \psi}{\cos \alpha} \geq \frac{-1}{\cos \alpha} > \frac{-2}{\sqrt{3}},
\]

hence (4) is true for this case. Now restrict to the case when \( \alpha < 0 \). Then \( 2 \cos(\psi - \alpha) < -1 \) and

\[
\frac{\cos \psi}{\cos \alpha} \geq -\frac{\cos(\pi + 2\alpha - \phi)}{\cos \alpha} > -1,
\]

hence (4) is true.
Claim (d). From the assumption there is some \( v = [\lambda; \delta] \in P^+ \) with \( \frac{\sqrt{3}}{2 \sin(\delta - \phi)} \leq \lambda \leq 1 \) and \( \delta \in [\frac{\pi}{2} - \bar{\phi}, \frac{\pi}{2}] \) such that

\[
u_j = T_n v = (\lambda \cos \delta - \cos \phi)e_1 + (\lambda \sin \delta - \sin \phi)e_2.
\]

We are done if we show that \( x_1 \) is chosen for the next step of the iteration, i.e. \( \chi_j = x_1 \). In this case

\[
u_{j+1} = \lambda \cos \delta e_1 + (\lambda \sin \delta - 2 \sin \phi)e_2.
\]

\( u_{j+1} \) has a smaller \( e_2 \)-coordinate than the original point \( v \in P^+ \), hence \( u_{j+1} \in R \cup Q \cup P^+ \). We are left with the mentioned claim and show that the argument angle \( \alpha_j \) of \( u_j \) satisfies \( \alpha_j \leq \pi - \phi \). From

\[
\lambda \sin(\phi + \delta) \geq \frac{\sqrt{3} \sin(\phi + \bar{\phi})}{2 \sin(\delta - \phi)} \geq \frac{\sqrt{3}}{2} > \sin 2\phi
\]

we get

\[
(\lambda \cos \delta - \cos \phi) \sin \phi \geq - \cos \phi(\lambda \sin \delta - \sin \phi).
\]

Since \( \lambda \sin \delta - \sin \phi > 0 \) and \( \sin \phi \geq 0 \) these terms does not change the type of inequality. We obtain

\[
\cot \alpha_j = \frac{\lambda \cos \delta - \cos \phi}{\lambda \sin \delta - \sin \phi} \geq - \cot \phi = \cot(\pi - \phi),
\]

which proves the desired fact. \( \square \)

Lemma 8. In the situation of Lemma 7 we have \( V \cap T = \emptyset \).

Proof. By construction \( (P \cup Q \cup R) \cap T = \emptyset \). By symmetry it is therefore enough to show that \( T_n(P^+) \cap T = \emptyset \). As before, let \( u = [\lambda; \delta] \in P^+ \), where \( \delta \in [\frac{\pi}{2} - \bar{\phi}, \frac{\pi}{2}] \) and \( \frac{\sqrt{3}}{2 \sin(\delta - \phi)} \leq \lambda \leq 1 \). Then

\[
T_n u = (\lambda \cos \delta - \cos \phi)e_1 + (\lambda \sin \delta - \sin \phi)e_2.
\]

Starting with

\[
\lambda \cos(\delta - \bar{\phi}) \leq \cos(\delta - \bar{\phi}) \leq \frac{\sqrt{3}}{2} \leq \cos(\phi - \bar{\phi}),
\]

expanding and dividing by \( \lambda \sin \delta - \sin \phi > 0 \) and by \( \cos \bar{\phi} > 0 \) we get

\[
\cot \arg T_n u = \frac{\lambda \cos \delta - \cos \phi}{\lambda \sin \delta - \sin \phi} \leq - \tan \bar{\phi} = \cot(\frac{\pi}{2} + \bar{\phi}),
\]

which shows that the argument angle of \( T_n u \) is greater or equal than \( \frac{\pi}{2} + \bar{\phi} \). Therefore \( T_n u \not\in T \), which proves the assertion. \( \square \)
Proof of Theorem 4. Again, the set \( A_{2,1} \) from Example 10 below shows that \( u^*_{2,1} \geq \sqrt{2} \). Moving \( e_1 \) slightly away from \( e_2 \) turns \( A_{2,1} \) into a balanced set and shows that also \( u^*_{2,2} \geq \sqrt{2} \). Hence it suffices to prove \( u^*_{2,1}, u^*_{2,2} \leq \sqrt{2} \). Contrarily, we assume that there exists an iteration such that \( \lambda_i > \sqrt{2} \) for some fixed \( i \in \mathbb{N} \). Without loss of generality we may assume that \( i \) is the smallest such index, in particular \( \lambda_{i-1} \leq \sqrt{2} \).

The angle \( \gamma_j \in [0, \pi] \) between \( u_j \) and \( \chi_j \) is defined for all \( j \in \mathbb{N} \) since without loss of generality we may assume \( u_j \neq 0 \). Now observe that

\[
\frac{\pi}{2} + \phi = \frac{1}{2}(2\pi - (\pi - 2\phi)) \leq \gamma_j \leq \pi
\]

for all \( j \in \mathbb{N} \). A simple computation yields

\[
\lambda_j^2 = 1 + 2\lambda_{j-1} \cos \gamma_{j-1} + \lambda_{j-1}^2.
\] (5)

Hence

\[
2\lambda_{i-1} \cos \gamma_{i-1} = \lambda_i^2 - \lambda_{i-1}^2 - 1 > 2 - 2 - 1 = -1,
\]

and

\[-\frac{1}{2} < -\frac{1}{2\lambda_{i-1}} < \cos \gamma_{i-1} \leq \cos \left( \frac{\pi}{2} + \phi \right) = -\sin \phi,
\]

since from (5) we also have \( 1 < \lambda_{i-1} \). Therefore

\[
\frac{\pi}{2} + \phi \leq \gamma_{i-1} \leq \frac{2}{3}\pi \quad \text{and} \quad 0 \leq \phi < \frac{\pi}{6}.
\]

In other words there is a gap greater than \( \frac{2}{3}\pi \) between two neighboring elements of \( X \). In a second step of the proof we will explore possible ranges of \( \alpha_{i-1} \). Clearly, the angle between \( u_{i-1} \) and \( x_1, x_n \) is less or equal than \( \frac{2}{3}\pi \). Therefore exactly one of the following cases holds.

Case 1. \( \alpha_{i-1} \in (\frac{\pi}{2} - \phi, \frac{\pi}{2} + \phi) \), where \( \phi := \frac{\pi}{6} - \phi \). Hence \( u_{i-1} \in T \) but also \( u_{i-1} \in V \) from Lemma 7. This contradicts Lemma 8.

Case 2. \( \alpha_{i-1} \in (\frac{3}{2}\pi - \phi, \frac{3}{2}\pi + \phi) \), where \( \phi := \frac{\pi}{6} + \phi \). We can restrict the range of \( \alpha_{i-1} \) further by adding the above condition not only for \( x_1 \) and \( x_n \), but for all elements of \( X \). Doing so we get that

\[
\begin{cases}
\frac{2}{3}\pi > \alpha_{i-1} - \phi_j, & \text{if } \pi \geq \alpha_{i-1} - \phi_j, \text{ and} \\
\frac{4}{3}\pi < \alpha_{i-1} - \phi_j, & \text{if } \pi < \alpha_{i-1} - \phi_j.
\end{cases}
\]

Let \( k = 1, \ldots, n - 1 \) be the greatest index satisfying \( \pi < \alpha_{i-1} - \phi_k \). Since \( k \) is maximal we have \( \pi \geq \alpha_{i-1} - \phi_{k+1} \). We get \( \phi_{k+1} - \phi_k > \frac{2}{3}\pi \), which shows that there must be a second gap which is greater than \( \frac{2}{3}\pi \). After a rotation of the coordinate system and renumbering the elements of \( X \) we may apply Lemma 8 again and obtain a contradiction.

The indirect assumption must have been wrong in Cases 1 and 2, hence both \( u^*_{2,1}, u^*_{2,2} \leq \sqrt{2} \). \( \square \)
3. Examples

This section provides examples illustrating that the situation is more complicated in dimension \( d \geq 3 \). All examples are unique up to rotation of \( \mathbb{R}^d \).

Example 9. For \( l \geq 1 \) we describe the operation of choosing \( l + 1 \) equidistant points \( x_0, \ldots, x_l \in S^{l-1} \subseteq \mathbb{R}^l \). Equidistant means that the value \( s \) of the scalar product does not depend on the chosen pair of points. Since all vectors have unit length, the constant scalar product equals \( \cos \alpha \) for some \( \alpha \in [0, \pi] \). By recursion on \( l \) suppose \( \tilde{x}_1, \ldots, \tilde{x}_l \) have been found in the next lower dimension \( l - 1 \), with scalar product \( \tilde{s} \). Set

\[
x_0 = (0, 0, \ldots, 0, 1), \quad x_1 = (\tilde{x}_1 \cos \alpha, \sin \alpha), \quad \ldots, \quad x_l = (\tilde{x}_l \cos \alpha, \sin \alpha).
\]

We demand

\[
\sin \alpha = \langle x_0, x_1 \rangle = s = \langle x_i, x_j \rangle = \sin^2 \alpha + \langle \tilde{x}_i, \tilde{x}_j \rangle \cos^2 \alpha,
\]

which leads to \( s = s^2 + (1 - s^2)\tilde{s} \). Solving this equation gives \( s = \frac{\tilde{s}}{1 - \tilde{s}} \). It is easy to see that the recursion produces the values

\[
-1, -\frac{1}{2}, -\frac{1}{3}, -\frac{1}{4}, \ldots
\]

for \( s \). Hence, when denoting the scalar product of dimension \( l \) by \( s_l \), we get \( s_l = s = -\frac{1}{l} \). Knowing \( s \) it is also clear that \( x_0 + \ldots + x_d = 0 \) since \( \tilde{x}_1 + \ldots + \tilde{x}_d = 0 \).

In low dimensions, equidistant points are just two points on the real line \( (l = 1) \), a regular triangle in a circle \( (l = 2) \), or a tetrahedron in a 2-sphere \( (l = 3) \).

Clearly, the set \( X \) of \( d + 1 \) equidistant points is balanced in \( S^{d-1} \subseteq \mathbb{R}^d \). The problem of finding \( u^*(X) \) in this case was approached by a computer experiment only. We checked \( d = 2, \ldots, 12 \) and found that \( u^*(X) = a(d) \frac{d}{d} \), where \( a \) is the integer sequence

\[
0, 1, 2, 4, 6, 9, 12, 16, 20, 25, 30, 36, 42, \ldots
\]

starting at index \( d = 0 \). Obviously, \( u_i \) may take only a certain finite number of values on the lattice

\[
\left\{ \sum_{i=1}^{d+1} k_i x_i \mid k_i \in \mathbb{N}_0 \right\},
\]

all of which are close to the origin. For example, there are 3 possibilities for \( d = 1 \) and 7 for \( d = 2 \). The sequence \( a \) has relations to other fields and problems [ATT]. Note also that \( a(d) < d\sqrt{d} \), or equivalently \( u^*(X) \leq \sqrt{d} \). The latter inequality was an ad-hoc conjecture for a general set \( X \), which turned out to be true only in dimension \( d = 2 \).
Example 10. For $1 \leq m \leq d$ consider the following set $X = A_{d,m}$ consisting of $n = d + m$ points. As before, let $e_i \in \mathbb{R}^d$ be the vector with all zero components except the $i$th which is 1. Then define

$$A_{d,m} := \{e_1, e_2, \ldots, e_d, -e_1, -e_2, \ldots, -e_m\}.$$ 

Proposition 11. Let $X = A_{d,m}$ be as in Example 10.

(i) $A_{d,m}$ is $m$-balanced,

(ii) $u^*(A_{d,m}) \geq \sqrt{d - m + 1}.$

Proof. (i) is clear from the definition; the origin is contained in the $m$-dimensional face of $\text{conv}(A_{d,m})$ spanned by $\pm e_1, \ldots, \pm e_m$. For (ii) observe that there is an iteration such that $u_i = e_{m+1} + e_{m+2} + \ldots + e_{m+i}$ for $1 \leq i \leq d - m$. 

It is likely that equality holds in (ii), but we do not need this stronger assertion.

Example 12. The following construction of $X = B_{d,b}(\epsilon, \phi)$ depends on the dimension $d$, some integer $1 \leq b \leq d - 2$, some real numbers $\epsilon > 0$ and $0 < \phi < \frac{\pi}{2}$, where the value of $\phi$ is uncritical. For $c := d - b$, $2 \leq c \leq d - 1$, we have the orthogonal decomposition $\mathbb{R}^d = \mathbb{R}^b \oplus \mathbb{R}^c$. The subspaces contain unit hyperspheres $S^{b-1} \subseteq \mathbb{R}^b$ and $S^{c-1} \subseteq \mathbb{R}^c$.

In $S^{c-1}$ choose $c+1$ points $x_0, x_1, \ldots, x_c$ as follows. Fix any direction $v \in S^{c-1}$ and consider the linear hyperplane $V$ which is perpendicular to $v$. In $S^{c-2} = V \cap S^{c-1}$ choose $c$ equidistant points $\bar{x}_1, \ldots, \bar{x}_c$ as described in Example 9. Then let

$$x_i := \cos(\epsilon) \bar{x}_i + \sin(\epsilon) v$$

for $i = 1, \ldots, c$. Note that $x_1, \ldots, x_c$ are equidistant in $S^{c-2}(\cos \epsilon) := (V + \sin(\epsilon) v) \cap S^{c-1}$. The remaining point $x_0$ is given by

$$x_0 := -\cos(\phi) x_1 + \sin(\phi) v.$$ 

In $S^{b-1}$ choose $b + 1$ equidistant points $x_{c+1}, \ldots, x_{d+1}$, which makes a total of $n = d + 2$ points in $X$.

Proposition 13. For $d \geq 3$ and $X = B_{d,b}(\epsilon, \phi)$ the following statements are true.

(i) $X$ is $b$-balanced,

(ii) for any large $M > 0$ there is an $\epsilon > 0$ such that $u^*(X) \geq \sqrt{M}$.

Proof. (i) is clear from the definition; the origin is contained in the $b$-dimensional face spanned by $x_{c+1}, \ldots, x_{d+1}$. Note that $x_1 + \ldots + x_c = c \sin(\epsilon) v$ and

$$\sigma := \langle x_i, x_j \rangle = \langle \bar{x}_i, \bar{x}_j \rangle \cos^2 \epsilon + \sin^2 \epsilon = 1 - \frac{c}{c-1} \cos^2 \epsilon$$

where $x_i = \cos(\epsilon) \bar{x}_i + \sin(\epsilon) v$ for $i = 1, \ldots, c$.
since \( \langle \bar{x}_i, \bar{x}_j \rangle = -\frac{1}{c-1} \) for all \( 1 \leq i, j \leq c \). From now on we suppose that \( \epsilon \) is sufficiently small such that
\[
- \frac{1}{c-1} < \sigma < 0.
\] (6)

We also have
\[
\langle x_0, x_i \rangle = \begin{cases} 
-\cos \phi + \sin \phi \sin \epsilon; & i = 1, \\
-\sigma \cos \phi + \sin \phi \sin \epsilon; & 1 < i \leq c.
\end{cases}
\]

To prove (ii), we show that the iteration which starts with \( x_0 \) and adds points from \( \{x_1, \ldots, x_c\} \) as long as possible is feasible. More precisely,
\[
u_0 = 0, \quad u_1 = x_0, \quad u_2 = x_0 + x_1, \ldots, \quad u_{c+1} = x_0 + x_1 + \cdots + x_c.
\]

In general for \( i = 0, 1, \ldots \) we can write
\[
u_{ic+1} = x_0 + (i-1)(x_1 + x_2 + \ldots + x_c), \\
u_{ic+2} = x_0 + (i-1)(x_1 + x_2 + \ldots + x_c) + x_1, \\
\vdots \\
u_{ic+c} = x_0 + (i-1)(x_1 + x_2 + \ldots + x_c) + (x_1 + x_2 + \ldots + x_{c-1}), \\
u_{(i+1)c+1} = x_0 + i(x_1 + x_2 + \ldots + x_c).
\] (7)

In what follows we fix \( 0 \leq i \leq k \) and \( 0 \leq j \leq c - 1 \) arbitrarily, and consider step \( s := (i + 1)c + j + 1 \) of the iteration (7). In other words, we want to control the iteration up to and including step \( (k + 1)c + m + 1 \), where \( 0 \leq m \leq c - 1 \).

(a) To be able to choose \( x_{j+1} \) in step \( s \) we must have
\[
\langle u_s, x_{j+1} \rangle \leq 0.
\]

(b) Also, to make the choice of \( x_{j+1} \) work, the scalar product with all other vectors must be at least as big as the one from (a), or
\[
\langle u_s, x_{l+1} \rangle \geq \langle u_s, x_{j+1} \rangle
\]
for all \( 0 \leq l \leq c - 1 \).

(c) The point \( x_0 \) must not come into play, which is the case when
\[
\langle u_s, x_0 \rangle \geq 0.
\]

(d) By construction we have
\[
\langle u_s, x_{r+1} \rangle = 0
\]
for \( c \leq r \leq d \).

Let us now analyze these conditions. There is nothing to show for (d). For (c) we compute
\[
\langle u_s, x_0 \rangle = \begin{cases} 
1 + ic \sin \epsilon \sin \phi; & j = 0, \\
1 - \cos \phi + ic \sin \epsilon \sin \phi - (j - 1)\sigma \cos \phi + j \sin \epsilon \sin \phi; & 0 < j \leq c - 1.
\end{cases}
\]
From this expression it is clear that (c) is always satisfied. Looking at (a) and (b) and observing that \(1 + (c - 1)\sigma = c \sin^2 \epsilon\) we compute

\[
\langle u_s, x_{j+1} \rangle = \begin{cases} 
  ic \sin^2 \epsilon - \cos \phi + \sin \phi \sin \epsilon; & j = 0, \\
  ic \sin^2 \epsilon + j\sigma - \sigma \cos \phi + \sin \phi \sin \epsilon; & 0 < j \leq c - 1
\end{cases}
\]

and for \(l \neq j\)

\[
\langle u_s, x_{l+1} \rangle = \begin{cases} 
  ic \sin^2 \epsilon + (j - 1)\sigma + 1 - \cos \phi + \sin \phi \sin \epsilon; & 0 = l < j, \\
  ic \sin^2 \epsilon + (j - 1)\sigma + 1 - \sigma \cos \phi + \sin \phi \sin \epsilon; & 0 < l < j, \\
  ic \sin^2 \epsilon + j\sigma - \sigma \cos \phi + \sin \phi \sin \epsilon; & l > j.
\end{cases}
\]

From these expressions (b) is immediately clear; one just has to compare the varying terms and to use (6). It remains to analyze Condition (a). For \(j = 0\) it can be expressed as

\[
i \leq \frac{\cos \phi - \sin \phi \sin \epsilon}{c \sin^2 \epsilon},
\]

for \(j > 0\) note that we have a set of \(c - 1\) inequalities, whose “sharpness” increases with \(j\), cf. (6). Therefore it suffices to take the last condition \((j = c - 1)\) which reads

\[
i \leq \frac{\sigma(\cos \phi - (c - 1)) - \sin \phi \sin \epsilon}{c \sin^2 \epsilon}.
\]

In the second and last part of the proof, the assertion is brought into play. Assume the length \(\sqrt{M}\) is reached in step \((k + 1)c + m + 1\), i.e.

\[
\|u_{(k+1)c+m+1}\|^2 \geq M.
\]

For arbitrary \(k\) and \(1 \leq m \leq c - 1\) we have

\[
\|u_{(k+1)c+m+1}\|^2 = 1 + (kc + 2m)kc \sin^2 \epsilon + (1 + (m - 1)\sigma)(m - 2 \cos \phi) + 2(kc + m) \sin \epsilon \sin \phi,
\]

while for \(m = 0\) we get the simpler expression

\[
\|u_{(k+1)c+1}\|^2 = 1 + k^2 c^2 \sin^2 \epsilon + 2kc \sin \epsilon \sin \phi.
\]

Assuming \(m = 0\) (to use the advantages of the simpler form) and inserting (11) into (10) we get an inequality which is quadratic in \(k\):

\[
k^2 + k \frac{2 \sin \phi}{c \sin \epsilon} + \frac{1 - M}{c \sin^2 \epsilon} \geq 0.
\]

Solving the inequality gives

\[
k \geq \frac{\sqrt{\sin^2 \phi - 1 + M} - \sin \phi}{c \sin \epsilon}.
\]

To finish the proof, we must put together (8) and (12) as well as (9) and (12). For the first pairing, solve

\[
\sqrt{\sin^2 \phi - 1 + M} - \sin \phi \leq \frac{\cos \phi - \sin \phi \sin \epsilon}{\sin \epsilon}.
\]
Isolating $M$ yields
\[ M \leq \cos^2 \phi \left( 1 + \frac{1}{\sin^2 \epsilon} \right). \]

For small $\epsilon$, the right-hand side becomes arbitrarily large, which finishes this part of the proof. For the remaining pairing, one has to solve
\[ \sqrt{\sin^2 \phi - 1 + M - \sin \phi} \leq \frac{\sigma (\cos \phi - (c - 1)) - \sin \phi \sin \epsilon}{\sin \epsilon}. \]

Isolating $M$ again gives
\[ M \leq \frac{\sigma^2 (\cos \phi - (c - 1))^2}{\sin^2 \epsilon} + \cos^2 \phi, \]

which with small $\epsilon$ again has an arbitrarily large right-hand side. \hfill \Box

**Example 14.** The following construction of a point set $X = C_d(\epsilon, \mu, \phi)$ depends on the dimension $d \geq 3$, on real numbers $\epsilon \geq 0$, $\mu > 0$ and $0 < \phi < \frac{\pi}{2}$, where the value of $\phi$ is uncritical. Pick any unit vector $v \in \mathbb{R}^d$ which determines a hyperplane $V$ of $\mathbb{R}^d$. In $S^{d-2} \subseteq V$ choose $d$ equidistant points $\bar{x}_1, \ldots, \bar{x}_d$ as described in Example 9. Then define
\[ x_i := \cos(\epsilon)\bar{x}_i - \sin(\epsilon) v \]
for $i = 1, \ldots, d$. The two remaining points are given by
\[ x_{d+1} = -\cos(\mu)\bar{x}_1 + \sin(\mu) v, \]
\[ x_0 = \cos(\phi)\bar{x}_1 + \sin(\phi) v. \]

Finally let $X := \{x_0, x_1, \ldots, x_d, x_{d+1}\}$.

**Proposition 15.** For $d \geq 3$ the following statements are true.

(i) $C_d(\epsilon, \mu, \phi)$ is $d$-balanced for $\epsilon > 0$, and $(d - 1)$-balanced for $\epsilon = 0$,
(ii) for any large $M > 0$ there is an $\epsilon > 0$ such that $u^*(C_d(\epsilon, 3\epsilon, \frac{\pi}{6})) \geq \sqrt{M}$,
(iii) for any large $M > 0$ there is a $\mu > 0$ such that $u^*(C_d(0, \mu, \frac{\pi}{6})) \geq \sqrt{M}$.

**Proof.** (i) is immediately clear from the definition, in particular for $\epsilon = 0$ the origin is contained in the $(d - 1)$-dimensional face spanned by $x_1, \ldots, x_d$. We are left with (ii) and (iii) which are shown simultaneously. Consider the following
finite piece of an iteration for $C_d(\epsilon, \mu, \phi)$. Start with $u_0 = 0$, and let

$$
\begin{align*}
  u_1 &= x_0, \\
  u_2 &= x_0 + x_{d+1}, \\
  u_3 &= x_0 + x_1 + x_{d+1}, \\
  &\vdots \\
  u_{2k-1} &= x_0 + (k-1)(x_1 + x_{d+1}), \\
  u_{2k} &= x_0 + (k-1)(x_1 + x_{d+1}) + x_{d+1}, \\
  u_{2k+1} &= x_0 + k(x_1 + x_{d+1}).
\end{align*}
$$

The following conditions (a)–(c) are sufficient for the iteration to work as above, up to step $2k + 1$.

(a) We must have $\langle u_l, x_0 \rangle \geq 0$ for all $1 \leq l \leq 2k + 1$, i.e. $x_0$ is never chosen between steps 2 and $2k + 1$ of the iteration.

(b) Additionally, also the scalar product with the other vector must be at least as big as the chosen one, meaning

$$
\langle u_{2i}, x_1 \rangle \leq \langle u_{2i}, x_{d+1} \rangle, \quad \langle u_{2i+1}, x_{d+1} \rangle \leq \langle u_{2i+1}, x_1 \rangle
$$

for all $1 \leq i \leq k$.

(c) To be able to choose $x_{d+1}$ in step $2i$ and $x_1$ in step $2i + 1$ we must have

$$
\langle u_{2i}, x_1 \rangle \leq \langle u_{2i}, x_m \rangle, \quad \langle u_{2i+1}, x_{d+1} \rangle \leq \langle u_{2i+1}, x_m \rangle,
$$

for all $1 \leq i \leq k$ and $2 \leq m \leq d$.

In order to examine Condition (a) it is straightforward to compute

$$
\langle u_l, x_0 \rangle = \begin{cases} 
  1 - \cos(\phi + \epsilon) + i \left( \cos(\phi + \epsilon) - \cos(\phi + \mu) \right); & l = 2i, \\
  1 + i \left( \cos(\phi + \epsilon) - \cos(\phi + \mu) \right); & l = 2i + 1.
\end{cases}
$$

Since $\mu > \epsilon$ for both (ii) and (iii), the terms on the right-hand side are always non-negative. Therefore (a) does not impose any additional condition. Similarly, for Condition (b) we compute

$$
\langle u_l, x_1 \rangle = \begin{cases} 
  \cos(\phi + \epsilon) - 1 + i \left( 1 - \cos(\mu - \epsilon) \right); & l = 2i, \\
  \cos(\phi + \epsilon) + i \left( 1 - \cos(\mu - \epsilon) \right); & l = 2i + 1.
\end{cases}
$$

$$
\langle u_l, x_{d+1} \rangle = \begin{cases} 
  \cos(\mu - \epsilon) - \cos(\phi + \mu) + i \left( 1 - \cos(\mu - \epsilon) \right); & l = 2i, \\
  -\cos(\phi + \mu) + i \left( 1 - \cos(\mu - \epsilon) \right); & l = 2i + 1,
\end{cases}
$$

which is equivalent to

$$
\begin{align*}
  \cos(\phi + \epsilon) - 1 &\leq \cos(\mu - \epsilon) - \cos(\phi + \mu), \\
  -\cos(\phi + \mu) &\leq \cos(\phi + \epsilon).
\end{align*}
$$
Again, since both inequalities are always true, (b) does not introduce new conditions either. Finally, Condition (c) requires
\[
\langle u_{2i}, x_m \rangle - \langle u_{2i}, x_1 \rangle = \frac{d}{d-1} \cos \epsilon \left( \cos \epsilon - \cos \phi + i(\cos \mu - \cos \epsilon) \right) \geq 0,
\]
\[
\langle u_{2i+1}, x_m \rangle - \langle u_{2i+1}, x_{d+1} \rangle = -\frac{d}{d-1} \cos \phi \cos \epsilon + \cos(\phi + \epsilon) + \cos(\phi + \mu) + \frac{d}{d-1}(\cos \mu - \cos \epsilon) \cos \epsilon \geq 0.
\]
We demand that if \( i \) satisfies the first inequality, then it shall also satisfy the second. This leads to the additional condition
\[
\frac{\cos \phi - \cos \epsilon}{\cos \mu - \cos \epsilon} \leq \frac{d}{d-1} \cos \phi \cos \epsilon - \cos(\phi + \epsilon) - \cos(\phi + \mu) \]
\[
- \frac{d}{d-1}(\cos \mu - \cos \epsilon) \cos \epsilon,
\]
which is satisfied if \( \frac{3}{4} \leq \cos \phi \), which is the reason for the choice of \( \phi = \frac{\pi}{6} \).

Summing up we are left with the condition
\[
i \leq \frac{\cos \phi - \cos \epsilon}{\cos \mu - \cos \epsilon}.
\] (13)

We can now finish the proof for (ii) and (iii). If the length \( \sqrt{M} \) is reached in step \( 2k + 1 \), then we have
\[
\|u_{2k+1}\|^2 = 1 + 2k(\cos(\phi + \epsilon) - \cos(\phi + \mu)) + 2k^2(1 - \cos(\mu - \epsilon)) \geq M.
\]
Solving the quadratic inequality in \( k \) and using standard trigonometric identities we get
\[
k \geq \frac{\sqrt{\sin^2(\phi + \mu + \epsilon) + M - 1 - \sin(\phi + \mu + \epsilon)}}{2 \sin \frac{\mu + \epsilon}{2}}.
\] (14)

Putting together (13) and (14) we get
\[
\frac{\cos \phi - \cos \epsilon}{\cos \mu - \cos \epsilon} \geq \frac{\sqrt{\sin^2(\phi + \mu + \epsilon) + M - 1 - \sin(\phi + \mu + \epsilon)}}{2 \sin \frac{\mu + \epsilon}{2}}.
\]

Finally we isolate \( M \) and arrive at
\[
M \leq \frac{(\cos \epsilon - \cos \phi)^2}{\sin^2 \frac{\mu + \epsilon}{2}} + \frac{2(\cos \epsilon - \cos \phi) \sin(\phi + \frac{\mu + \epsilon}{2})}{\sin \frac{\mu + \epsilon}{2}} + 1.
\]

For (ii) replace \( \mu \) by \( 3\epsilon \), for (iii) set \( \epsilon = 0 \). In both cases the right-hand side becomes arbitrarily large when \( \epsilon \) resp. \( \mu \) approaches zero. \( \square \)
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[FIG] Animated version of Figure 1, see http://www.math.tu-berlin.de/~tbinder/animation.gif.

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