# 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

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

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 $\operatorname{argmin}_{x \in X} \langle x, u_i \rangle$). 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 $\mathrm{SEB}(\tilde{Y})$ of $\tilde{Y}$ exists and is unique [Wel91]. We assume that $\tilde{Y}$ has at least two elements. By

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$c \in \mathbb{R}^d$ and $R \in \mathbb{R}^+$ we denote center and radius of $\mathrm{SEB}(\tilde{Y})$, respectively. Bădoiu and Clarkson [BC03] introduced the following approximation of $c$:

$$c_0 := 0, \qquad c_{i+1} := c_i + \frac{1}{i+1}(\xi_i - c_i), \tag{1}$$

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

$$\tilde{X} := \left\{ \frac{1}{R}(y - c) \;\middle|\; y \in \tilde{Y} \right\}. \tag{2}$$

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 $\mathrm{SEB}(\tilde{Y})$, 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 $\mathrm{SEB}(\tilde{Y})$. 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 $i \in \mathbb{N}$

$$\frac{\|c - c_i\|}{R} \leq \frac{1}{\sqrt{i}}. \tag{3}$$

[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* $\mathrm{SEB}(\tilde{Y})$*. Then for all $i \in \mathbb{N}$*

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

*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) $\mathrm{SEB}(X) = S^{d-1}$,
(ii) *The origin $0 \in \mathbb{R}^d$ is contained in* $\mathrm{conv}(X)$,
(iii) $\delta(X) \geq 0$, *where*

$$\delta(X) := -\max_{\|u\|=1} \min_{x \in X} \langle x, u \rangle.$$

*Proof.* (i)$\Longleftrightarrow$(ii) is due to R. Seidel (cf. Lemma 1 in [FGK03]). (ii)$\Longleftrightarrow$(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 $u$. $\square$

$X$ is called 0-balanced if $0 \notin \operatorname{conv}(X)$. For $1 \leq b \leq d-1$ the set $X$ is called $b$-balanced, if 0 is a point 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 $i \in \mathbb{N}_0$. $\square$

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

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

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. $\square$

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

$$\|u_i\| \leq \frac{1}{2\delta(X)} + 1, \qquad i \in \mathbb{N}_0.$$

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 $\mathrm{SEB}(\tilde{Y})$. Then $\|c - c_i\| \leq \frac{\sqrt{2}R}{i}$ 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

$$\begin{aligned} \chi_j &= \cos(\psi_j)\, e_1 + \sin(\psi_j)\, e_2 = [1; \psi_j], \\ u_j &= \lambda_j \big(\cos(\alpha_j)\, e_1 + \sin(\alpha_j)\, e_2\big) = [\lambda_j; \alpha_j]. \end{aligned}$$

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 $\mathcal{T}_k(W)$ denote the set obtained by translation of $W$ by $x_k$. The set $T$ is defined by

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

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

$$\begin{aligned} R &:= \{ [\tilde{r}; \tilde{\phi}] \mid \tilde{r} > 0 \text{ and } \tilde{\phi} \in (\pi - \phi, 2\pi + \phi) \}, \\ Q &:= \{ (a, b) \mid |a| \tan\phi \leq b \leq |a| \tan\phi + \lambda_{min} \}, \\ P &:= \{ u \in \mathbb{R}^2 \mid \|u\| \leq 1 \} \setminus (R \cup Q). \end{aligned}$$

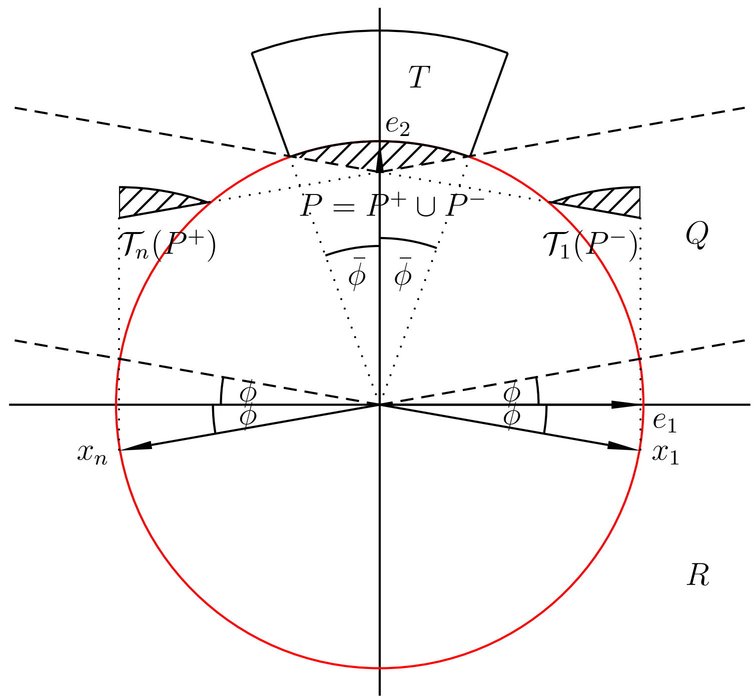
Here $\lambda_{min} := \frac{\sqrt{3}}{2\cos\phi}$ is the length of the intersection of $Q$ with the $e_2$-axis. Figure 1 gives an illustration of this situation; [FIG] gives an animated version where $\phi$ varies in time.

**Lemma 7.** *Let $X$ be a finite subset of $S^1 \subseteq \mathbb{R}^2$, parametrized as above. Suppose that $\phi \in [0, \frac{\pi}{6})$, i.e. the size of the base gap is greater than $\frac{2}{3}\pi$. Define the set $V$ by*

$$V := P \,\cup\, \mathcal{T}_n(P^+) \,\cup\, \mathcal{T}_1(P^-) \,\cup\, Q \,\cup\, R,$$

*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 $\phi$, $\mathcal{T}_1(P^-) \setminus (Q \cup R)$ and $\mathcal{T}_n(P^+) \setminus (Q \cup R)$ 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 $u_{j+1} \in \mathcal{T}_n(P^+) \cup \mathcal{T}_1(P^-)$.
(c) If $u_j \in R$, then $u_{j+1} \in P \cup Q \cup R$.
(d) If $u_j \in \mathcal{T}_n(P^+)$, then $u_{j+1} \in P \cup Q \cup R$.
(e) If $u_j \in \mathcal{T}_1(P^-)$, 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 $\mathcal{T}_1(Q)$ and $\mathcal{T}_n(Q)$ 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 $\lambda_{min} = \frac{\sqrt{3}}{2\cos\phi}$ (which denotes the length of the intersection of $Q$ with the $e_2$-axis) and dividing by $\cos\phi > 0$ we get

$$(\lambda \sin\alpha + \sin\psi) - \lambda_{min} < \tan\phi\,(\lambda\cos\alpha + \cos\psi).$$

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

$$u_j = \mathcal{T}_n v = (\lambda \cos\delta - \cos\phi)e_1 + (\lambda \sin\delta - \sin\phi)e_2.$$

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

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

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 $\sin\phi \geq 0$ division by 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. □

**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 $\mathcal{T}_n(P^+) \cap T = \emptyset$. 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

$$\mathcal{T}_n u = (\lambda \cos\delta - \cos\phi)e_1 + (\lambda \sin\delta - \sin\phi)e_2.$$

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

$$\cot \arg \mathcal{T}_n u = \frac{\lambda\cos\delta - \cos\phi}{\lambda\sin\delta - \sin\phi} \leq -\tan\bar{\phi} = \cot\Big(\frac{\pi}{2} + \bar{\phi}\Big),$$

which shows that the argument angle of $\mathcal{T}_n u$ is greater or equal than $\frac{\pi}{2} + \bar{\phi}$. Therefore $\mathcal{T}_n u \notin T$, which proves the assertion. □

*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

$$\lambda_j^2 = 1 + 2\lambda_{j-1} \cos \gamma_{j-1} + \lambda_{j-1}^2. \tag{5}$$

Hence

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

and

$$-\frac{1}{2} < -\frac{1}{2\lambda_{i-1}} < \cos \gamma_{i-1} \leq \cos\Big(\frac{\pi}{2} + \phi\Big) = -\sin \phi,$$

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

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

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

**Case 2.** $\alpha_{i-1} \in (\frac{3}{2}\pi - \bar{\bar{\phi}}, \frac{3}{2}\pi + \bar{\bar{\phi}})$, where $\bar{\bar{\phi}} := \frac{\pi}{6} + \phi$. 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 $k = 1, \dots, n-1$ 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 $u^*(X) = \frac{a(d)}{d}$, 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

$$\Big\{ \sum_{i=1}^{d+1} k_i x_i \;\Big|\; k_i \in \mathbb{N}_0 \Big\},$$

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 $1 \le m \le d$ 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

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

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

(i) *$A_{d,m}$ is $m$-balanced,*
(ii) *$u^*(A_{d,m}) \ge \sqrt{d - m + 1}$.*

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

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 $1 \le b \le d - 2$, some real numbers $\epsilon > 0$ and $0 < \phi < \frac{\pi}{2}$, where the value of $\phi$ is uncritical. For $c := d - b$, $2 \le c \le d - 1$, 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 $x_0, x_1, \dots, x_c$ 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 $\bar{x}_1, \dots, \bar{x}_c$ as described in Example 9. Then let

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

for $i = 1, \dots, c$. Note that $x_1, \dots, x_c$ 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 $x_{c+1}, \dots, x_{d+1}$, which makes a total of $n = d + 2$ points in $X$.

**Proposition 13.** *For $d \ge 3$ 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 $u^*(X) \ge \sqrt{M}$.*

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

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

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

$$-\frac{1}{c-1} < \sigma < 0. \tag{6}$$

We also have

$$\langle x_0, x_i \rangle = \begin{cases} -\cos\phi & +\sin\phi \sin\epsilon; \quad i = 1, \\ -\sigma\cos\phi & +\sin\phi\sin\epsilon; \quad 1 < i \leq c. \end{cases}$$

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,

$$u_0 = 0, \qquad u_1 = x_0, \qquad u_2 = x_0 + x_1, \quad \ldots, \quad u_{c+1} = x_0 + x_1 + \cdots + x_c.$$

In general for $i = 0, 1, \ldots$ we can write

$$\begin{aligned} u_{ic+1} &= x_0 + (i-1)(x_1 + x_2 + \ldots + x_c), \\ u_{ic+2} &= x_0 + (i-1)(x_1 + x_2 + \ldots + x_c) + x_1, \\ &\vdots \\ u_{ic+c} &= x_0 + (i-1)(x_1 + x_2 + \ldots + x_c) + (x_1 + x_2 + \ldots + x_{c-1}), \\ u_{(i+1)c+1} &= x_0 + i(x_1 + x_2 + \ldots + x_c). \end{aligned} \tag{7}$$

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

$$\langle u_s, x_{j+1}\rangle = \begin{cases} i\,c\sin^2\epsilon - \cos\phi & +\sin\phi\sin\epsilon; \quad j = 0, \\ i\,c\sin^2\epsilon + j\sigma - \sigma\cos\phi & +\sin\phi\sin\epsilon; \quad 0 < j \le c-1 \end{cases}$$

and for $l \neq j$

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

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

$$i \le \frac{\cos\phi - \sin\phi\sin\epsilon}{c\sin^2\epsilon}, \tag{8}$$

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

$$i \le \frac{\sigma(\cos\phi - (c-1)) - \sin\phi\sin\epsilon}{c\sin^2\epsilon}. \tag{9}$$

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.

$$\|u_{(k+1)c+m+1}\|^2 \ge M. \tag{10}$$

For arbitrary $k$ and $1 \le m \le c-1$ we have

$$\begin{aligned} \|u_{(k+1)c+m+1}\|^2 \quad &= \quad 1 + (kc+2m)kc\sin^2\epsilon + \big(1 + (m-1)\sigma\big)(m - 2\cos\phi) + \\ &\quad\quad 2(kc+m)\sin\epsilon\sin\phi, \end{aligned}$$

while for $m = 0$ we get the simpler expression

$$\|u_{(k+1)c+1}\|^2 = 1 + k^2c^2\sin^2\epsilon + 2kc\sin\epsilon\sin\phi. \tag{11}$$

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

$$k^2 + k\frac{2}{c}\frac{\sin\phi}{\sin\epsilon} + \frac{1-M}{c^2\sin^2\epsilon} \ge 0.$$

Solving the inequality gives

$$k \ge \frac{\sqrt{\sin^2\phi - 1 + M} - \sin\phi}{c\sin\epsilon}. \tag{12}$$

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

$$\sqrt{\sin^2\phi - 1 + M} - \sin\phi \le \frac{\cos\phi - \sin\phi\sin\epsilon}{\sin\epsilon}.$$

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. □

**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

$$\begin{aligned} x_{d+1} &= -\cos(\mu)\bar{x}_1 + \sin(\mu)\, v, \\ x_0 &= \cos(\phi)\bar{x}_1 + \sin(\phi)\, v. \end{aligned}$$

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

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

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

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

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

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

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

which is equivalent to

$$\begin{aligned}
\cos(\phi+\epsilon) - 1 &\leq \cos(\mu-\epsilon) - \cos(\phi+\mu), \\
-\cos(\phi+\mu) &\leq \cos(\phi+\epsilon).
\end{aligned}$$

Again, since both inequalities are always true, (b) does not introduce new conditions either. Finally, Condition (c) requires

$$\begin{aligned}\langle u_{2i}, x_m\rangle - \langle u_{2i}, x_1\rangle &= \frac{d}{d-1}\cos\epsilon\big(\cos\epsilon - \cos\phi + i(\cos\mu - \cos\epsilon)\big) \;\geq\; 0,\\ \langle u_{2i+1}, x_m\rangle - \langle u_{2i+1}, x_{d+1}\rangle &= -\frac{d}{d-1}\cos\phi\cos\epsilon + \cos(\phi+\epsilon) + \cos(\phi+\mu) + \\ &\qquad i\,\frac{d}{d-1}(\cos\mu - \cos\epsilon)\cos\epsilon \;\geq\; 0.\end{aligned}$$

We demand that if $i$ satisfies the first inequality, then it shall also satisfy the second. This leads to the additional condition

$$\frac{\cos\phi - \cos\epsilon}{\cos\mu - \cos\epsilon} \leq \frac{\frac{d}{d-1}\cos\phi\cos\epsilon - \cos(\phi+\epsilon) - \cos(\phi+\mu)}{\frac{d}{d-1}(\cos\mu - \cos\epsilon)\cos\epsilon},$$

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

$$i \leq \frac{\cos\phi - \cos\epsilon}{\cos\mu - \cos\epsilon}. \tag{13}$$

We can now finish the proof for (ii) and (iii). If the length $\sqrt{M}$ is reached in step $2k+1$, then we have

$$\|u_{2k+1}\|^2 = 1 + 2k\big(\cos(\phi+\epsilon) - \cos(\phi+\mu)\big) + 2k^2\big(1 - \cos(\mu-\epsilon)\big) \geq M.$$

Solving the quadratic inequality in $k$ and using standard trigonometric identities we get

$$k \geq \frac{\sqrt{\sin^2(\phi + \frac{\mu+\epsilon}{2}) + M - 1} - \sin(\phi + \frac{\mu+\epsilon}{2})}{2\sin\frac{\mu-\epsilon}{2}}. \tag{14}$$

Putting together (13) and (14) we get

$$\frac{\cos\phi - \cos\epsilon}{\cos\mu - \cos\epsilon} \geq \frac{\sqrt{\sin^2(\phi + \frac{\mu+\epsilon}{2}) + M - 1} - \sin(\phi + \frac{\mu+\epsilon}{2})}{2\sin\frac{\mu-\epsilon}{2}}.$$

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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