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Maximizing the maximum degree in ordered nearest neighbor graphs ☆

Péter Ágoston [a], Adrian Dumitrescu [b], Arsenii Sagdeev [c,*], Karamjeet Singh [d], Ji Zeng [e,a]

[a] Alfréd Rényi Institute of Mathematics, Budapest, Hungary
[b] Algoresearch L.L.C., Milwaukee, WI, USA
[c] Karlsruhe Institute of Technology, Karlsruhe, Germany
[d] Indraprastha Institute of Information Technology, Delhi, India
[e] University of California San Diego, La Jolla, CA, USA

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ABSTRACT

For an ordered point set in a Euclidean space or, more generally, in an abstract metric space, the *ordered Nearest Neighbor Graph* is obtained by connecting each of the points to its closest predecessor by a directed edge. We show that for every set of n points in $\mathbb{R}^d$, there exists an order such that the corresponding ordered Nearest Neighbor Graph has maximum degree at least $\log n/(4d)$. Apart from the $1/(4d)$ factor, this bound is the best possible. As for the abstract setting, we show that for every n-element metric space, there exists an order such that the corresponding ordered Nearest Neighbor Graph has maximum degree $\Omega(\sqrt{\log n/\log\log n})$.

1. Introduction

For a given point set P in the plane, in d-dimensional Euclidean space, or, even more generally, in an arbitrary metric space, its *Nearest Neighbor Graph* is a directed graph based on minimum distances. More precisely, these points are the vertices of the Nearest Neighbor Graph, and each vertex has precisely one outgoing edge towards its closest neighbor. To make this notion well-defined, we assume that our point set is in *general position*, which here means that no three points determine an isosceles triangle.

These graphs play an important role in modern Computational Geometry due to their relevance in the context of computing geometric shortest paths [16,17]. Further applications of Nearest Neighbor Graphs for computing spanners, well-separated pairs, and approximate minimum spanning trees in $\mathbb{R}^d$ can be found in the survey [21], books [10,19], or monograph [18], see also [14]. A systematic study of the basic combinatorial properties of Nearest Neighbor Graphs dates back at least to the classical paper [13] by Eppstein, Paterson, and Yao in which, among many other results, they made the following simple observation: two edges with the same endpoint meet at an angle of at least $\pi/3$. Hence, the maximum indegree of the Nearest Neighbor Graph of a point set $P \subset \mathbb{R}^d$ is bounded from above by the *kissing number* of $\mathbb{R}^d$, see [8], i.e., the maximum number of non-overlapping unit spheres that can touch a unit sphere in $\mathbb{R}^d$, regardless of the size of P.

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* Corresponding author.
E-mail addresses: agostonp95@gmail.com (P. Ágoston), ad.dumitrescu@algoresearch.org (A. Dumitrescu), sagdeevarsenii@gmail.com (A. Sagdeev), karamjeets@iiitd.ac.in (K. Singh), jzeng@ucsd.edu (J. Zeng).

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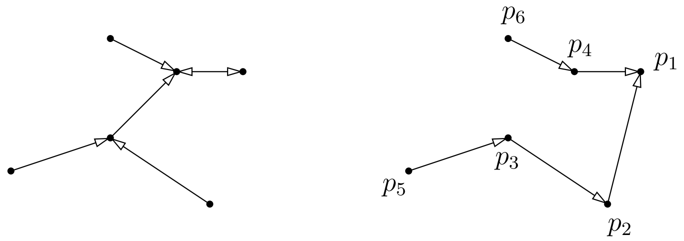

Fig. 1. Unordered (left) and ordered (right) Nearest Neighbor Graphs on the same set of six points.

Here we extend the latter result and study the maximum indegree in a closely related class of *ordered Nearest Neighbor Graphs* introduced in [1,11] in the context of dynamic algorithms. In this case, the vertices appear one by one, and each new vertex has precisely one outgoing edge towards its closest predecessor, see Fig. 1.

It is not hard to see that every point set admits an order such that the corresponding ordered Nearest Neighbor Graph is a path, and thus its maximum indegree is 1 (Proposition 1). We therefore focus on a 'dual' problem, where the goal is to construct an order that *maximizes* the maximum indegree. We have the following results, partially addressing this question in three different settings.

For n points on the line, the maximum indegree can be made $\lceil \log n \rceil$, which is optimal. (Unless specified otherwise, all logarithms in this paper are in base 2.)

Theorem 1. *For every set of n points on the line, there exists an order such that the corresponding ordered Nearest Neighbor Graph has maximum indegree at least $\lceil \log n \rceil$. On the other hand, there is a set of n points on the line such that for every order, the indegree of each point is at most $\lceil \log n \rceil$.*

We obtain a similar maximum indegree (with a loss factor $1/(4d)$) for n points in $\mathbb{R}^d$, and in view of Theorem 1, this bound is best possible apart from the loss factor.

Theorem 2. *For every set of n points in $\mathbb{R}^d$, there exists an order such that the corresponding ordered Nearest Neighbor Graph has maximum indegree at least $\log n/(4d)$.*

The maximum indegree we manage to obtain in a metric space on n points is only about $\sqrt{\log n}$, and closing the gap between this lower bound and the $\lceil \log n \rceil$ upper bound remains as a challenging open problem.

Theorem 3. *For every n-element metric space, there exists an order such that the corresponding ordered Nearest Neighbor Graph has maximum indegree $\Omega\left(\sqrt{\log(n)/\log\log(n)}\right)$.*

Related work For a point set in the plane, the notion of (ordered or unordered) Nearest Neighbor Graph admits the following generalization. The space around each point is divided into k cones of equal angle similarly positioned around each point, and each point is connected to a 'nearest' neighbor in each cone. Depending on the definition of 'nearest' (either in a sense of the Euclidean distance or in terms of the projection on the cones' bisectors), the resulting graph is called either a *Yao* or a *Theta Graph*. These notions were introduced by Yao [22] and Clarkson [9], respectively, and their ordered variants are due to Bose, Gudmundsson, and Morin [5]. These graphs are useful in constructing spanners with nice additional properties, such as logarithmic maximum degree and logarithmic diameter that are obtained for suitable insertion orders, see also [12]. Sparse graphs with a small dilation have been studied in [3,5–7], among others.

Note that the special case $k = 1$ retrieves the original definition of the (ordered) Nearest Neighbor Graph. However, for larger k, it is an open problem in the field to determine whether every point set P admits an order such that the maximum indegree of the corresponding ordered Yao or Theta Graph is bounded from above by some constant c_k, independent of the size of P, see [5]. To get a better understanding of how degrees behave in these graphs, here we attempt to *maximize* the maximum indegree. The general case $k \geq 2$ will be addressed in a subsequent paper.

In contrast, constructing an order *minimizing* the maximum indegree of the ordered Nearest Neighbor Graph is rather straightforward.

Proposition 1. *For every point set P, there is an order such that the corresponding ordered Nearest Neighbor Graph is a path. Moreover, any point in P can be chosen to be the tail of this path.*

Proof. Write $n = |P|$ and fix an arbitrary point $p_n \in P$. For $1 \leq i \leq n-1$, let p_{n-i} be the point closest to p_{n-i+1} among the points $P \setminus \{p_n, p_{n-1}, \dots, p_{n-i+1}\}$. Now consider the order $\pi = (p_1, p_2, \dots, p_n)$. It is easy to check that the ordered Nearest Neighbor Graph G corresponding to π is just the path $p_n \to p_{n-1} \to \ldots \to p_1$. Indeed, at the moment when p_i is introduced, we connect p_i to the point among $\{p_1, p_2, \dots, p_{i-1}\}$ that is closest to p_i, which is exactly p_{i-1} according to our construction of π. □

Notation. For a finite point set $P \subset \mathbb{R}^d$, we use $\mathrm{diam}(P)$ to denote its diameter, i.e., the maximum distance between any pair of points in P, and $\mathrm{conv}(P)$ to denote its convex hull.

2. Points on the line: proof of Theorem 1

Upper bound. We construct the desired set of points on the line recursively. For $n = 2^1$, we put $P = P_1 = \{0, 1\}$. For $k \geq 1$ and $n = 2^{k+1}$, we put $P = P_{k+1} = P_k \cup (3^k + P_k)$. It is straightforward to verify by induction that $\mathrm{diam}(P_k) = (3^k - 1)/2$, which is smaller than the distance between the two 'halves' of P_{k+1}, namely, P_k and $3^k + P_k$. Indeed, $\mathrm{diam}(P_k) = (3^k - 1)/2 < (3^k + 1)/2$. Therefore, in every order of P_{k+1}, each point can have at most one edge incoming from the other 'half'. Hence by induction, the indegree of each point does not exceed $k + 1 = \log n$. Finally, if $2^k < n \leq 2^{k+1}$, then an arbitrary subset $P \subseteq P_{k+1}$ of size n inherits the latter property.

Lower bound. Choose k such that $\lceil \log n \rceil = k+1$, i.e., $2^k < n \leq 2^{k+1}$. The proof is by induction on k. Note that the statement is trivial for $k = 0$, so let us now assume that $k \geq 1$. We identify a suitable subset $P' \subseteq P$ such that its reveal already forces the indegree of one of the points to reach the required threshold. The remaining points in $P \setminus P'$ are introduced afterwards and clearly do not decrease any degree. We may assume that P lies on the x-axis. Let $X \subseteq P$. We outline a recursive procedure Order for generating a suitable order that employs the following subroutines and a distinguished element of P:

- Center(X): refers to a specified element of X that has a high indegree (to be determined). If $X = \{x\}$, then Center(X) $= x$.
- Order(X): lists the elements of X in a suitable order that ensures the existence of Center(X). Moreover, Center(X) appears first in this order.
- AnyOrder(X): lists the elements of X in an arbitrary order; for instance from left to right.
- Delete(L, x): deletes x from list L and returns the resulting list.

Algorithm Order(P)

Step 1: Let a and b denote the leftmost and rightmost points of P.
Step 2: Partition $P = A \cup B$ around the midpoint of ab: let A be the set of points of P that are closer to a than to b (including a itself), while B is the set of remaining points; assume without loss of generality that $|A| \geq |B|$; if $|A| < |B|$ proceed analogously by switching A with B and a with b.
Step 3: List P as follows: Center(A), b, Delete(Order(A), Center(A)), AnyOrder($B \setminus \{b\}$).
Step 4: Center(P) $\leftarrow$ Center(A).

Analysis Let $\Delta^-(P)$ denote the indegree of Center(P). Note that Order(A) is a list obtained by a recursive call and that the distance from b to A is strictly larger than the diameter of A by construction. Therefore, the indegree of Center(A) is increased by 1 due to the directed edge $b \to$ Center(A) that is added when b is revealed to the algorithm as the second point. As a result,

$$\Delta^-(P) \geq \Delta^-(A) + 1 \geq k + 1,$$

where the last inequality holds by induction hypothesis since $2^{k-1} < |A|$. □

3. Points in $\mathbb{R}^d$: proof of Theorem 2

Here we further develop the ideas from the previous subsection to translate them from the line to $\mathbb{R}^d$, for any fixed d. As the main supplementary tool, we use the following standard result in discrete geometry, that can be deduced, e.g., from [20, Ineq. (4) and (6)], see also [4]

Theorem 4. *Let K be a convex set in $\mathbb{R}^d$, K_0 be its interior, and $r < 1$ be a positive number. Then K can be covered by at most $(1 + 1/r)^d (d \ln d + d \ln \ln d + 5d)$ translates of $-rK_0$, reflected scaled copies of K_0.*

Corollary 1. *Let P be a finite set of points in $\mathbb{R}^d$ such that* $\mathrm{diam}(P) \leq 1$. *Then P can be partitioned into at most $16^d/2$ subsets of diameter less than* $1/2$.

Proof. We apply Theorem 4 with $K = \mathrm{conv}(P)$ and $r = 1/2$. Note that $\mathrm{diam}(K) = \mathrm{diam}(P) \leq 1$, and thus the distance between any two points of $-(1/2)K_0$ is *strictly less* than $1/2$. It remains only to note that the number of translates given by Theorem 4 is smaller than $16^d/2$ for all $d \geq 2$. □

Now we construct the desired order of P with large maximum indegree of the corresponding ordered Nearest Neighbor Graph by the following algorithm, which is a higher-dimensional extension of the procedure we used in Section 2.

Algorithm Order(P)

Step 1: Compute a diameter pair ab, where we may assume that $|ab| = 1$.
Step 2: Let $A = \{p \in P : |pa| \le |pb|\}$, and $B = \{p \in P : |pb| \le |pa|\}$. Assume w.l.o.g. that $|A| \ge |B|$, thus $|A| \ge n/2$.
Step 3: By Corollary 1, partition A into at most $16^d/2$ subsets where each subset has diameter less than $1/2$. One of these subsets $C \subseteq A$ contains at least $n/16^d$ points.
Step 4: List P in the following order:

$$\text{Center}(C), b, \text{Delete}(\text{Order}(C), \text{Center}(C)), \text{AnyOrder}\big(P \setminus (C \cup \{b\})\big).$$

Step 5: Center(P) ← Center(C)

Analysis Order(P) is a list obtained by a recursive call. Observe that in Order(P), the element Center(P) is listed first, as required. As earlier, let $\Delta^-(P)$ denote its indegree. By construction, the indegree of Center(C) is increased by 1 due to the directed edge $b \to \text{Center}(C)$ that is added when b is revealed to the algorithm as the second point. Moreover, for each subsequent step that reveals an element $c \in C$, since $\text{diam}(C) < 1/2$ and $|cb| \ge 1/2$, C is processed in a manner independent of the presence of b. As a result,

$$\Delta^-(P) \ge \Delta^-(C) + 1.$$

We now show that $\Delta^-(P) \ge \log_{16^d} n = \log n/(4d)$. This inequality is clearly satisfied for $n = 1, 2$. By induction, it is verified that

$$\Delta^-(P) \ge \Delta^-(C) + 1 \ge \log_{16^d}(n/16^d) + 1 = \log n/(4d) - 1 + 1 = \log n/(4d). \qquad \square$$

4. Abstract metric spaces: proof of Theorem 3

Let ρ be a metric on a finite set $V = \{v_1, \ldots, v_n\}$, namely a positive and symmetric function $\rho : V \times V \to \mathbb{R}_+$ satisfying the triangle inequality. So far we labeled the points of V arbitrarily just for definiteness, the desired order on them will be constructed later. We assume familiarity with hypergraphs, otherwise readers are referred to [15] for related definitions.

We define a 3-coloring of a complete 3-uniform hypergraph $K_n^{(3)}$ on the vertex set $[n]$ as follows: for all $1 \le i_1 < i_2 < i_3 \le n$, we color the triple $\{i_1, i_2, i_3\}$ by red (resp. green or blue) whenever $v_{i_2}v_{i_3}$ (resp. $v_{i_1}v_{i_3}$ or $v_{i_1}v_{i_2}$) is the 'shortest side' of a triangle $v_{i_1}v_{i_2}v_{i_3}$, that is $\rho(v_{i_2}, v_{i_3}) < \rho(v_{i_1}, v_{i_2})$ and $\rho(v_{i_2}, v_{i_3}) < \rho(v_{i_1}, v_{i_3})$. Recall that our points are in general position, meaning that no point triple determines an isosceles triangle, and so each triple gets exactly one color. A subhypergraph of $K_n^{(3)}$ is *monochromatic* if all its triples are of the same color. A *forward star* $S_k^{(3)}$ is a 3-uniform hypergraph on an ordered vertex set $\{i_1, \ldots, i_k\} \subseteq [n]$, labeled in the ascending order, consisting of edges $\{i_1, i_j, i_{j'}\}$ for all $i_j < i_{j'}$. We claim that if there exists a red clique $K_k^{(3)}$, or a green forward star $S_k^{(3)}$, or a blue forward star $S_k^{(3)}$, then there exists an order such that the corresponding Nearest Neighbor Graph has maximum indegree at least $k - 1$. To verify this claim, suppose that such a structure exists on the vertex set $I = \{i_1, \ldots, i_k\}$, labeled in the ascending order, and consider the following three cases.

First, suppose that these vertices form a red clique. We claim that under the order

$$v_{i_k}, v_{i_1}, v_{i_2}, \ldots, v_{i_{k-1}}, \text{AnyOrder}(V \setminus I),$$

the indegree of v_{i_k} is at least $k - 1$. Indeed, note that as each new vertex v_{i_j} is revealed, $\rho(v_{i_j}, v_{i_k})$ is the shortest distance among all currently visible points. Hence, $v_{i_j} \to v_{i_k}$ is an edge of the ordered Nearest Neighbor Graph for all $1 \le j \le k-1$.

Similarly, if these vertices form a blue forward star, then the indegree of v_{i_1} under the order

$$v_{i_1}, v_{i_k}, v_{i_{k-1}}, \ldots, v_{i_2}, \text{AnyOrder}(V \setminus I),$$

is at least $k - 1$. Indeed, when v_{i_j} is revealed, the distance $\rho(v_{i_1}, v_{i_j})$ will be the shortest among all current points as $\{i_1, i_j, i_\ell\}$ is always blue.

Finally, if these vertices form a green forward star, then the indegree of v_{i_1} under the order

$$v_{i_1}, v_{i_2}, v_{i_3}, \ldots, v_{i_k}, \text{AnyOrder}(V \setminus I),$$

is at least $k - 1$. Indeed, when v_{i_j} is revealed, an arbitrary currently visible point v_{i_ℓ} satisfies $\{i_1, i_\ell, i_j\}$ being green. So the distance $\rho(v_{i_1}, v_{i_j})$ will be the shortest.

The last ingredient of the proof is the following Ramsey-type result due to He and Fox; more precisely, their Theorem 1.2 and Lemma 5.2 in [15]. We rewrite this proof to make it explicit that the argument in [15] produces forward stars and also extends to more than two colors.

Theorem 5. *Let $K_n^{(3)}$ be a complete 3-uniform hypergraph on an ordered vertex set $[n]$, and its edges be colored by either red, green, or blue. If $K_n^{(3)}$ contains neither a red clique $K_k^{(3)}$, nor a green forward star $S_k^{(3)}$, nor a blue forward star $S_k^{(3)}$, then $n \le \exp\left(O\left(k^2 \log(k)\right)\right)$.*

Applying this theorem with $k = c'\sqrt{\log(n)/\log\log(n)}$ for a sufficiently small $c' > 0$, we ensure the existence of a monochromatic special structure, and thus the existence of an order such that the corresponding ordered Nearest Neighbor Graph has maximum indegree at least $k-1$, which completes the proof of Theorem 3.

Proof of Theorem 5. We consider a process of picking and deleting vertices from $V(K_n^{(3)})$, and constructing an auxiliary graph G. We keep track of two sets U, the vertex set of G, and W, the set of vertices waiting to be picked. At the beginning of the process, we have $U = \emptyset$ and $W = V(K_n^{(3)}) = [n]$. In each iteration, we pick the smallest vertex $v \in W$, and delete it from W. Then, following a rule we shall describe, we create edges from v to vertices in U, assign v a color (red/green/blue), and add it into U. During this step, immediately after we created an edge $\{u, v\}$, we look at every vertex $w \in W$: if at least $|W|/k$ vertices w satisfy that $\{u, v, w\}$ is green, then we color the edge $\{u, v\}$ green (and vertex v green, see further below), and delete all $w \in W$ with $\{u, v, w\}$ not green; otherwise, we perform the same checking, coloring, and deleting with "blue" in place of "green"; if neither of these cases happens, we color the edge $\{u, v\}$ by red, and delete all $w \in W$ such that $\{u, v, w\}$ is not red.

Now we describe how we create edges: once a new vertex v is picked, we keep creating edges from v to the red vertices in U following the order until we encounter a green or blue edge; if the last edge we created is green (resp. blue), we color the vertex green (resp. blue); otherwise we color this vertex red. The new vertex and the created edges are considered as added into G. By construction, every edge in G leads to a red vertex and each green (resp. blue) vertex is adjacent to exactly one green (resp. blue) edge. The next iteration begins as long as there are still vertices left in W.

If there are k red vertices in G, then by construction all the 2-edges between them are red. And again by the way we color the edges in G, these vertices correspond to a 3-uniform red clique $K_k^{(3)}$ inside $K_n^{(3)}$. Hence, without loss of generality, we may assume that there are fewer than k red vertices in G. Given this assumption, if there are $(k-1)^2$ green vertices in G, then by our construction and the pigeonhole principle, there must be one red vertex v_1 and $k-1$ green vertices $v_2, \ldots, v_k$ such that $\{v_1, v_i\}$ is green for $2 \le i \le k$. Then by the way we color the edges in G, these vertices correspond to a 3-uniform green forward star $S_k^{(3)}$ inside $K_n^{(3)}$. Hence, without loss of generality, there are fewer than $(k-1)^2$ green vertices in G, and a similar claim holds for blue vertices as well. Therefore, G has fewer than $k + 2(k-1)^2$ vertices in total.

Next, we upper bound the number of edges in G. Since green edges only originate from green vertices, there are fewer than $(k-1)^2$ green edges. Similarly, there are fewer than $(k-1)^2$ blue edges. There are at most $(k-1)^2$ red edges between red vertices. To count other red edges, notice that the i-th red vertex has fewer than $k-1$ green (resp. blue) edges adjacent to it, and each endpoint of these edges is adjacent to $i-1$ red edges. In summary, the number of red edges in G is fewer than

$$(k-1)^2 + \sum_{i=1}^{k-1} (i-1)(k-1) = k(k-1)^2/2.$$

Finally, notice that each vertex in G decreases the size of W by 1, each green or blue edge preserves at least a $1/k$-fraction of the elements of W and each red edge preserves at least a $(1-2/k)$-fraction of the elements of W. Since by the end of our construction of G when W is depleted, G has fewer than $k + 2(k-1)^2$ vertices, fewer than $2(k-1)^2$ green or blue edges, and fewer than $k(k-1)^2/2$ red edges, the size of W in the beginning, namely n, is at most

$$(k + 2(k-1)^2)(1/k)^{-2(k-1)^2}(1-2/k)^{-k(k-1)^2/2} \le \exp\left(O\left(k^2 \log(k)\right)\right).$$

Here, we used an elementary estimate that $(1-2/k)^{-k/2} < e^2$. □

5. Concluding remarks

Recall from the second half of Theorem 1 that there exists a set of n points on the line such that for every order, the indegree of each point in the corresponding Nearest Neighbor Graph is at most $\lceil \log n \rceil$. Unlike the linear case, we do not know if this construction is close to being tight for larger dimensions or abstract metric spaces.

Note that both in the definition of Nearest Neighbor Graph corresponding to a metric space and in our proof of Theorem 3, we didn't really use the triangle inequality, and thus we could argue in a more general setting of *semimetric spaces*. Moreover, the *exact* distances between the points are also not important, since only their *relative order* determines the Nearest Neighbor Graph. Furthermore, we know from [2] that any order of the distances on an n-element set can be realized in the $(n-1)$-dimensional Euclidean space. Hence, a sufficiently strong improvement upon the result of Theorem 2 could strengthen the lower bound from Theorem 3 as well.

Observe that our proof of Theorem 3 works without any changes if instead of a red clique, we could guarantee only a red 'backward star', which is a much sparser hypergraph. (A *backward star* is a 3-uniform hypergraph similar to a forward star, where the only difference is that the common vertex of all the hyperedges has not the smallest, but the largest index.) We are unaware of any variant of Theorem 5 that guarantees a backward star in one color or a forward star in (one of) the other color(s) for a much smaller n. Note that the proof of Theorem 5 works for *any* coloring of the complete hypergraph, while colorings that come from metric spaces satisfy additional constraints due to transitivity.[1]

A closely related problem is the following:

Problem 1. For an n-element metric space V and $v \in V$, let $d(v)$ be the maximum indegree of v in the ordered Nearest Neighbor Graph over all $n!$ possible orders. Can $\sum_v 2^{-d(v)}$ be larger than 1?

On the one hand, note that if the sum $\sum_v 2^{-d(v)}$ is at most one, then $d(v) \geq \lceil \log n \rceil$ for at least one $v \in V$, which would strongly improve upon the result of Theorem 3. On the other hand, if $\sum_v 2^{-d(v)} > 1$ for some V, then all the points of an appropriate 'iterated blow-up' Q of V satisfy $d(q) < c \log |Q|$ for some $c < 1$ and all $q \in Q$, and this would improve the aforementioned upper bound from the second half of Theorem 1.

We managed to verify the inequality $\sum_v 2^{-d(v)} \leq 1$ for all $n \leq 5$ by computer search. Moreover, it is not hard to check that this sum equals exactly 1 for the metric spaces constructed in the second half of the proof of Theorem 1, and that these are not the only examples. However, computer experiments suggest that such metric spaces become rare as n grows. This can be tentatively considered as evidence towards a negative resolution of Problem 1.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data availability

No data was used for the research described in the article.

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[1] For instance, in the notation of Section 4, it is not possible that two triples $\{1,2,3\}$ and $\{1,3,4\}$ are blue, while $\{1,2,4\}$ is green, because otherwise we would have $v_1v_2 < v_1v_3 < v_1v_4 < v_1v_2$, a contradiction.

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