Characterization of finite metric spaces by their isometric sequences

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Introduction (Warming Up)

We put distinct four points x_1, x_2, x_3, x_4 on the Euclidean space $\mathbb{R}^2$.

Clearly, $1 \leq |\{d(x_i, x_j) \mid 1 \leq i < j \leq 4\}| \leq \binom{4}{2} = 6$.
But, the first equality does not hold.

Q1. Can we put x_1, x_2, x_3, x_4 on $\mathbb{R}^2$ such that
$2 = |\{d(x_i, x_j) \mid 1 \leq i < j \leq 4\}|$?

Q2. What else?

Q3. Can we find all of them up to similarity?

Q4. Can we put x_1, x_2, x_3, x_4 on $\mathbb{R}^3$ such that
$1 = |\{d(x_i, x_j) \mid 1 \leq i < j \leq 4\}|$?

Q5. Can we put x_1, x_2, x_3, x_4, x_5 on $\mathbb{R}^2$ such that
$2 = |\{d(x_i, x_j) \mid 1 \leq i < j \leq 4\}|$?

Distance Sets

A subset X of a Euclidean space is called an s-**distance set** if $|A(X)| = s$ where $A(X) = \{d(x, y) \mid x, y \in X, x \neq y\}$.

Problem

Given s, d, n, find all $X \subseteq \mathbb{R}^d$ such that $|A(X)| = s$ and $|X| = n$ up to similarity.

D.G.Larman, C.Rogers, J.J.Seidel

On two-distance sets in Euclidean space, Bull. London Math. Soc. 9 (1977), no. 3, 261-267.

E.Bannai, Et.Bannai, D.Stanton

An upper bound for the cardinality of an s-distance subset in real Euclidean space II, Combinatorica 3 (1983), no. 2, 147-152.

If $X \subseteq \mathbb{R}^d$ and $|A(X)| = s$, then $|X| \leq \binom{d+s}{s}$.

Not only distances but also triangles

Isometry

Let (X, d) be a metric space where $d : X \times X \to \mathbb{R}_{\geq 0}$ is a metric function. For $A, B \subseteq X$ we say that A is **isometric** to B if there exists a bijection $f : A \to B$ such that $d(x, y) = d(f(x), f(y))$ for all $x, y \in A$.

For a positive integer k we denote the family of k-subsets of X by $\binom{X}{k}$, and we define $A_k(X)$ to be the quotient set of $\binom{X}{k}$ by isometry, i..e,

$$A_k(X) = \left\{ [Y] \mid Y \in \binom{X}{k} \right\}$$

where $[Y] = \{Z \subseteq X \mid Z \text{ is isometric to } Y\}$.

Notation

$A_2(X)$ are identified with $\{d(x, y) \mid x, y \in X, x \neq y\}$.

Isometric Sequence

If X is a finite set, then we define the **isometric sequence** of (X, d) to be $(a_1, a_2, \ldots, a_n)$ where $a_i = |A_i(X)|$ and $|X| = n$.

In Euclidean spaces

(1) The four vertices in a square has the isometric sequence $(1, 2, 1, 1)$.

(2) The five vertices in a regular pentagon: $(1, 2, 2, 1, 1)$.

(3) The four vertices in a non-square rectangle: $(1, 3, 1, 1)$.

A connected graph is a metric space with the graph distance.

(4) The complete bipartite graph $K_{3,3}$: $(1, 2, 2, 2, 1, 1)$.

(5) The cycle C_6 : $(1, 3, 3, 3, 1, 1)$.

(6) The cocktail party graph $K_{2,2,2}$: $(1, 2, 2, 2, 1, 1)$.

Isometric sequences are obtained from
the partition $\{E_\alpha\}_{\alpha \in A_2(X)}$ of $\binom{X}{2}$ where $E_\alpha = \{\{x, y\} \mid d(x, y) = \alpha\}$.

(7) The discrete partition of $\binom{X}{2}$: $(1, \binom{n}{2}, \binom{n}{3}, \ldots, 1)$

What we can see from a given isometric sequence

From $(1, 2, 1, 1)$ we can see the following:

(1) $|X| = 4$ since the length of the sequence is four.

(2) All 3-subsets are isometric.

(3) $\{x, y, z\}$ is not a regular triangle but an isosceles triangle since $a_2 = 2$.

(4) If $d(x, y) = d(y, z) \neq d(x, z)$ and $w \notin \{x, y, z\}$, then $d(x, w) = d(w, z)$ and $d(y, z) = d(x, z)$.

(5) Thus, the partition of $\binom{\{x,y,z,w\}}{2}$ is uniquely determined up to permutations of X.

How to embed into a Euclidean space

Distance matrix

The matrix $\sum_{\alpha \in A_2(X)} \alpha^2 A_\alpha$ is called the **distance matrix** of (X, d) where A_α is the adjacency matrix of the graph (X, E_α).

On embeddings into Euclidean spaces we have the following criterion:

A.Neumaier

Distance matrices, dimension, and conference graphs, Nederl. Akad. Wetensch. Indag. Math. 43 (1981), no. 4, 385-391.

Setting $G := -(I - \frac{1}{n}J)(\sum_{\alpha \in A_2(X)} \alpha^2 A_\alpha)(I - \frac{1}{n}J)$,
if G is positive semidefinite,
then there exists an isometry from X to $\mathbb{R}^d$ where $d = \mathrm{rank}(G)$.

Example with $(1, 2, 1, 1)$

The following is the distance matrix D where $a = d(x, z)^2$ and $b = d(x, y)^2$:

$$D = \begin{pmatrix} 0 & a & b & b \\ a & 0 & b & b \\ b & b & 0 & a \\ b & b & a & 0 \end{pmatrix}, \det(tI - G) = t(t - a)^2(t - 2b + a)$$

We have $a \leq 2b$ iff G is positive semi-definite, and
the equality holds iff X is embedded into $\mathbb{R}^2$.

In general, we are required to find $A_2(X)$ such that G is positive semidefinite and $\mathrm{rank}(G)$ is minimal.

Trivial or Non-Trivial?

(1) $a_k = 1$ implies that all k-subsets of X are isometric.
Clearly, $a_1 = a_n = 1$ where $n = |X|$, and
if $\bigcap_\alpha \mathrm{Aut}(X, E_\alpha)$ is transitive on X, then $a_{n-1} = 1$.

Do you think whether it is trivial that $a_k = 1$ implies $a_2 = 1$?

(2) $a_k = 2$ implies that exactly two isometry classes exists in $\binom{X}{k}$.
Any graph and its complement induce a metric space with $a_2 = 2$, and every complete bipartite graph with at least five vertices induces a metric space with $a_2 = a_3 = 2$.

Is it trivial to characterize all metric spaces with $a_4 = 2$?

(3) A non-square rectangle has the isometric sequence $(1, 3, 1, 1)$.

Is it trivial that $a_2 \leq a_3$ if $n \geq 5$?

(4) The orbitals of $C_2 \wr (C_2 \wr C_2)$ on eight points satisfies $a_2 = a_3 = 3$.

Is it trivial to classify all metric spaces with $a_2 = a_3 = 3$?

In our main theorem we deal with the following isometric sequences $(a_1, a_2, \ldots, a_n)$:

1. $a_k = 1$ for some k with $2 \leq k \leq n-2$;
2. $a_k = 2$ for some k with $4 \leq k \leq \frac{-3+\sqrt{1+4n}}{2}$;
3. $a_3 = 2$ and $n \geq 5$;
4. $a_2 = a_3 = 3$ and $n \geq 5$.

Theorem 1 (H, Shinohara)

Let (X, d) be a finite metric space with its isometric sequence $(a_1, a_2, \ldots, a_n)$. If $a_k = 1$ for some k with $2 \leq k \leq n-2$, then $a_1 = a_2 = \cdots = a_n = 1$.

Theorem 2 (H, Shinohara)

Let (X, d) be a finite metric space with its isometric sequence $(a_1, a_2, \ldots, a_n)$. If $a_k = 2$ for some k with $4 \leq k \leq \frac{-3+\sqrt{1+4n}}{2}$, then $a_2 = 2$, and for some $\alpha \in A_2(X)$ the graph (X, E_α) is isomorphic to $K_{1,n-1}$ or $K_n \setminus K_2$.

Theorem 3 (H, Shinohara)

Let (X, d) be a finite metric space with its isometric sequence $(a_1, a_2, \ldots, a_n)$. If $a_3 = 2$ and $n \geq 5$, then $a_2 = 2$ and for some $\alpha \in A_2(X)$ (X, E_α) is isomorphic to a matching on X, a complete bipartite graph or the pentagon.

Theorem 4 (H, Shinohara)

Let (X, d) be a finite metric space with its isometric sequence $(a_1, a_2, \ldots, a_n)$. If $a_2 = a_3 = 3$ and $n \geq 5$, then $(X, \{E_\delta\}_{\delta \in A_2(X)})$ is isomorphic to one of the following:

Example 1

Let $\{Y, Z\}$ be the bipartition of $K_{4,4}$, and denote $K_{4,4}$ by (X, E_α). Let E_γ denote a complete matching on X which does not intersect with E_α, and E_β denote the complement of $E_\alpha \cup E_\gamma$. For each subset Y of X, if $|Y| \geq 5$, then $A_3(Y) = \{\alpha\alpha\beta, \alpha\alpha\gamma, \beta\beta\gamma\}$.

Example 2

Let $\{Y, Z\}$ be a bipartition of X. We define $E_\alpha = \binom{Y}{2} \cup \binom{Z}{2}$, E_γ to be a matching between Y and Z and E_β to be the complement of $E_\alpha \cup E_\beta$. Then $A_3(X) = \{\alpha\alpha\alpha, \alpha\beta\gamma, \beta\beta\alpha\}$.

Example 3

Let (X, E_β) and (X, E_γ) be matchings on X such that $(X, E_\beta \cup E_\gamma)$ is also a matching on X, and E_α the complement of $E_\beta \cup E_\gamma$. Then $A_3(X) = \{\alpha\alpha\alpha, \alpha\alpha\beta, \alpha\alpha\gamma\}$.

Example 4

Let $\{Y, Z\}$ be a bipartition of X with $|Z| = 2$. We define $E_\alpha = \binom{Y}{2}$, $E_\gamma = \binom{Z}{2}$ and E_β to be the complement of $E_\alpha \cup E_\gamma$. Then $A_3(X) = \{\alpha\alpha\alpha, \beta\beta\alpha, \beta\beta\gamma\}$.

Before going to prove

Let (X, d) be a finite metric space. For $A, B \subseteq X$ we define a vector $v(A, B)$ whose entries are indexed by the elements of $A_2(X)$ as follows:

$$v(A, B)_\alpha := |(A \times B) \cap R_\alpha|$$

where $R_\alpha := \{(x, y) \in X \times X \mid d(x, y) = \alpha\}$.

Lemma 1

(i) $v(A, B) = v(B, A)$;
(ii) If $A \cap B = \emptyset$, then $v(A \cup B, C) = v(A, C) + v(B, C)$;
(iii) $v(X, X)_\alpha = |R_\alpha| = 2|E_\alpha|$;
(iv) If A is isometric to B, then $v(A, A) = v(B, B)$;
(v) $|\{v(A, A) \mid A \in \binom{X}{k}\}| \leq a_k$;
(vi) For $B \in \binom{X}{k-1}$ we have $|\{v(x, B) \mid x \in X \setminus B\}| \leq a_k$,

Lemma 2

For distinct $\alpha, \beta \in A_2(X)$ and $A, B \in \binom{X}{k}$, if the induced subgraph of (X, E_α) by A contains a spanning star and that of (X, E_β) by B contains a spanning star, then A is not isometric to B.

For a positive integer k we define
$M_k := \{\alpha \in A_2(X) \mid \exists x \in X; v(x, X)_\alpha \geq k\}$,
so that $M_k \subseteq M_{k-1}$ for each k.

Lemma 3

Let $\alpha \in A_2(X) \setminus M_{k-1}$ and $A \in \binom{X}{k}$ such that the induced subgraph of (X, E_α) by A contains a spanning forest. If $k^2 - k \leq n$, then the number of edges in the forest is at most $a_k - 1$.

Proof of Theorem 1

Theorem 1 If $a_k = 1$ for some k with $2 \leq k \leq n-2$, then $a_2 = 1$.

- Suppose $a_2 > 1$, i.e., $\exists x, y, z \in X; d(x,y) \neq d(y,z)$;
- Set $\alpha := d(x,y)$ and $\beta := d(y,z)$;
- Let $w \in X \setminus \{x,y,z\}$ and $S \in \binom{X}{k-2}$ with $x, y, z, w \notin S$;
- Set $S_1 := S \cup \{x,y\}$, $S_2 := S \cup \{x,z\}$, $S_3 := S \cup \{y,z\}$, $S_4 := S \cup \{w,z\}$, so that $\forall i, S_i \in \binom{X}{k}$;
- For $u \in \{x,y,z,w\}$ we set $r(u) := v(u,S)_\alpha$.
- Applying Lemma 1 for $v(S_i, S_i)$ we obtain
  $r(x) + r(y) + 1 = r(x) + r(w) + v(x,w)_\alpha$,
  $r(y) + r(z) = r(z) + r(w) + v(w,z)_\alpha$,
- and hence, $1 \leq 1 + v(z,w)_\alpha = v(x,w)_\alpha \leq 1$.
- This implies that $d(x,w) = \alpha$.
- Similarly, we have $d(y,w) = \beta$.
- Since S_1 is not isometric to S_3, we have a contradiction to $a_k = 1$.

Sketch of the Proof of Theorem 2

Theorem 2 If $a_k = 2$ for some k with $4 \leq k \leq \frac{-3+\sqrt{1+4n}}{2}$, then $a_2 = 2$, and for some $\alpha \in A_2(X)$ the graph (X, E_α) is isomorphic to $K_{1,n-1}$ or $K_n \setminus K_2$.

- $|A_2(X) \setminus M_{k-1}| \leq 1$ by Lemma 3;
- If $A_2(X) \setminus M_{k-1} = \{\beta\}$, then $|E_\beta| = 1$ by Lemma 3;
  - By Lemma 2, $|M_{k-1}| \leq a_k = 2$, so $a_2 = 2$;
  - For $\alpha \in M_{k-1}$ we have $(X, \alpha) \simeq K_n \setminus K_2$.
- If $A_2(X) \setminus M_{k-1} = \emptyset$, then $M_2 = A_2(X)$;
  - By Lemma 2, $|M_{k-1}| \leq a_k = 2$, so $A_2(X) = \{\alpha, \beta\}$;
  - We may assume $\alpha \in M_{k+1}$ since $(k-1) + k + 1 \leq n$;
  - $\exists x \in X$; $|R(x)| \geq k + 1$;
  - For all $A, B \in \binom{R(x)}{k-1}$, $A \cup \{x\}$ is isometric to $B \cup \{x\}$;
  - It means that A is isometric to B since each permutation of $A \cup \{x\}$ which fixes the vertices of degree less than $k-1$ is an isometry.

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- By Lemma 2, $|M_{k-1}| \leq a_k = 2$, so $A_2(X) = \{\alpha, \beta\}$;
- We may assume $\alpha \in M_{k+1}$ since $(k-1) + k + 1 \leq n$;
- $\exists x \in X$; $|R(x)| \geq k+1$;
- For all $A, B \in \binom{R(x)}{k-1}$, $A \cup \{x\}$ is isometric to $B \cup \{x\}$;
- It means that A is isometric to B since each permutation of $A \cup \{x\}$ which fixes the vertices of degree less than $k-1$ is an isometry;
- By Theorem 1, $|A_2(R(x))| = 1$, so $A_2(R(x)) = \{\alpha\}$ or $\{\beta\}$;
- We rename $\beta \in A_2(X)$ so that (X, E_β) contains a clique of size $k+1$;
- Let Y be a clique of maximal size in (X, E_β);
- Then $(y, z) \in R_\alpha$ for each $z \in X \setminus Y$, and each $y \in Y$.
- By Lemma 1, $|X \setminus Y| = 1$, and hence $(X, E_\alpha) \simeq K_{1,n-1}$.

Outline of Poof of Theorem 3

Theorem 3 If $a_3 = 2$ and $n \geq 5$, then $a_2 = 2$ and for some $\alpha \in A_2(X)$ (X, E_α) is isomorphic to a matching on X, a complete bipartite graph or the pentagon.

- $a_2 \leq a_3 = 2$ by observation for the adjacency of five points;
- $A_2(X) = \{\alpha, \beta\}$;
- We have to choose two of $\{\alpha\alpha\alpha, \beta\beta\beta, \alpha\alpha\beta, \beta\beta\alpha\}$ to form $A_3(X)$;
- If (X, E_α) and (X, E_β) is triangle-free, then $n \leq 5$ since the Ramsey number $R(3,3) = 6$. In this case (X, E_α) is the pentagon.
- Suppose (X, E_α) contains a triangle, so that $\alpha\alpha\alpha \in A_2(X)$;
- The number of connected components of (X, E_α) is at most two, otherwise $\beta\beta\beta, \beta\beta\alpha \in A_3(X)$, a contradiction;
- If it is two, then each connected component of (X, E_α) is a clique, so that (X, E_β) is complete bipartite;
- If it is one, then $\alpha\alpha\beta \in A_3(X)$ since (X, E_α) is not complete;
- This implies that (X, E_β) is a matching on X.

Ideas to prove Theorem 4

Theorem If $a_2 = a_3 = 3$ and $n \geq 5$, then $(X, \{E_\delta\}_{\delta \in A_2(X)})$ is isomorphic to one of the following:

- Suppose $A_3(X) = \{\alpha, \beta, \gamma\}$;
- $A_3(X) \subseteq \{\alpha\alpha\alpha, \beta\beta\beta, \gamma\gamma\gamma, \alpha\alpha\beta, \beta\beta\gamma, \gamma\gamma\alpha, \alpha\alpha\gamma, \gamma\gamma\beta, \beta\beta\alpha, \alpha\beta\gamma\}$;
- Suppose each of (X, E_α), (X, E_β), (X, E_γ) is triangle-free.
  - If (X, E_α) has a vertex of degree at least three, then $A_3(X) = \{\alpha\alpha\beta, \alpha\alpha\gamma, \beta\beta\gamma\}$ for a suitable ordering of β and γ.
  - If each of the three graph has no vertex of degree at least three, then $n - 1 \leq 2 + 2 + 2$, and we can prove that such case does not occur by hand.
- We may assume that $\alpha\alpha\alpha \in A_3(X)$;
- We claim that (X, E_β) or (X, E_γ) is a matching on X;

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- We claim that (X, E_β) or (X, E_γ) is a matching on X;
  - Otherwise, $\beta\beta\delta, \gamma\gamma\epsilon \in A_3(X)$ for some $\delta \in \{\alpha, \gamma\}$ and $\epsilon \in \{\alpha, \beta\}$;
  - This implies that (X, E_α) is a disjoint union of cliques;
  - Then $\beta\beta\alpha \in A_3(X)$ or $\gamma\gamma\alpha \in A_3(X)$;
  - We may assume $\beta\beta\alpha \in A_3(X)$.
  - $(X, E_\alpha \cup E_\beta)$ is a disjoint union of cliques;
  - This implies $\gamma\gamma\alpha, \gamma\gamma\beta \in A_3(X)$, a contradiction.
- We claim that, if each of (X, E_β) and (X, E_γ) is a matching, then $A_3(X) = \{\alpha\alpha, \alpha\alpha\beta, \alpha\alpha\gamma\}$ for a suitable ordering of β and γ.;
- We claim that, if (X, E_γ) is a matching but not so (X, E_β), then $A_3(X) = \{\alpha\alpha\alpha, \beta\beta\alpha, \alpha\beta\gamma\}$ $A_3(X) = \{\alpha\alpha\alpha, \beta\beta\alpha, \beta\beta\gamma\}$;
  - There are more cases to check than before. But, the used method is similar.

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- By the claims, for a suitable ordering of α, β, γ, $A_3(X)$ is one of the following:
- $\{\alpha\alpha\beta, \alpha\alpha\gamma, \beta\beta\gamma\}$;
- $\{\alpha\alpha\alpha, \alpha\beta\gamma, \beta\beta\alpha\}$;
- $\{\alpha\alpha\alpha, \alpha\alpha\beta, \alpha\alpha\gamma\}$;
- $\{\alpha\alpha\alpha, \beta\beta\gamma, \beta\beta\alpha\}$;
- $A_3(X)$ would give enough information to determine the structure of $(X, \{E_\alpha, E_\beta, E_\gamma\})$.

Thank you for your attention.