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Gromov product structures, quadrangle structures and split metric decompositions for finite metric spaces

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ABSTRACT

Let (X, d) be a finite metric space with elements P_i, $i = 1, \ldots, n$ and with distances $d_{ij} := d(P_i, P_j)$ for $i, j = 1, \ldots, n$. The "Gromov product" Δ_{ijk}, is defined as $\Delta_{ijk} = \frac{1}{2}(d_{ij} + d_{ik} - d_{jk})$. (X, d) is called Δ-generic, if, for each fixed i, the set of Gromov products Δ_{ijk} has a unique smallest element, $\Delta_{ij_ik_i}$. The Gromov product structure on a Δ-generic finite metric space (X, d) is the map that assigns the edge $E_{j_ik_i}$ to P_i. A finite metric space is called "quadrangle generic", if for all 4-point subsets $\{P_i, P_j, P_k, P_l\}$, the set $\{d_{ij}+d_{kl}, d_{ik}+d_{jl}, d_{il}+d_{jk}\}$ has a unique maximal element. The "quadrangle structure" on a quadrangle generic finite metric space (X, d) is defined as a map that assigns to each 4-point subset of X the pair of edges corresponding to the maximal element of the sums of distances. Two metric spaces (X, d) and (X, d') are said to be Δ-equivalent (Q-equivalent), if the corresponding Gromov product (quadrangle) structures are the same up to a permutation of X. We show that Gromov product classification is coarser than the metric fan classification. Furthermore it is proved that: (i) The isolation index of the 1-split metric δ_i is equal to the minimal Gromov product at the vertex P_i. (ii) For a quadrangle generic (X, d), the isolation index of the 2-split metric δ_{ij} is nonzero if and only if the edge E_{ij} is a side in every quadrangle whose set of vertices includes P_i and P_j. (iii) For a quadrangle generic (X, d), the isolation index of an m-split metric $\delta_{i_1 \ldots i_m}$ is nonzero if and only if any edge $E_{i_k i_l}$ is a side in every quadrangle whose vertex set contains P_{i_k} and P_{i_l}. These results are applied to construct a totally split decomposable metric for $n = 6$.

1. Introduction

The understanding of finite metric spaces is an interesting issue by several respects (the most important being probably the phylogenetic analysis) and the main device for classifying them is the so-called metric fan, which we will recall below in Section 2. As there are too many sub-cones of the metric cone constituting the metric fan (for example 194160 sub-cones coming in 339 symmetry classes for a 6-point space), coarser classifications seem to be desirable. In a previous paper [2] we presented an equivalence class decomposition of finite metric spaces using the set of minimal Gromov products at each point of that space. We recall the definitions and some results concerning Gromov product structures.

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Let (X, d) be a finite metric space with n elements P_i, $i = 1, \ldots, n$ ($n \geq 3$) and let d_{ij} be the distance between P_i and P_j. Since a finite metric space can be considered as a weighted complete graph, the elements of X are also referred to as "vertices" or "nodes". In this line, E_{ij} and T_{ijk} denote respectively an edge and a triangle with corresponding vertices.

Definition 1. The quantity Δ_{ijk}, defined as

$$\Delta_{ijk} = \Delta_{ikj} = \frac{1}{2}(d_{ij} + d_{ik} - d_{jk}), \tag{1}$$

is called the Gromov product of the triangle T_{ijk} at the vertex P_i. We call a metric space Δ-generic, if for each P_i the set of Gromov products Δ_{ijk} has a unique minimal element.

The quantity Δ_{ijk} is attributed to M. L. Gromov since it originates from his work on δ-hyperbolic metric spaces [5, Page 27].

By the triangle inequality, the Gromov products Δ_{ijk} are non-negative numbers. The distances d_{ij} can be expressed in terms of the Gromov products as

$$d_{ij} = \Delta_{ijk_1} + \Delta_{jik_1} = \Delta_{ijk_2} + \Delta_{jik_2} = \cdots = \Delta_{ijk_{n-2}} + \Delta_{jik_{n-2}}, \tag{2}$$

where the indices k_l run from 1 to n, excluding i and j, leading to a total of $n - 2$ equalities for each d_{ij}. In [2], we proved that a metric space can be defined using the Gromov products Δ_{ijk} as the primary ingredients in the sense that given a collection of Δ_{ijk} satisfying certain properties, then a metric space can be defined using Eq. (2), which produces the given collection of Δ_{ijk}.

The Gromov product structure for a Δ-generic finite metric space is defined as follows [2]:

Definition 2. Let (X, d) be a Δ-generic finite metric space. Let $P_i \in X$, and let $\Delta_{ij_ik_i}$ be the minimal Gromov product at P_i, ($i = 1, \ldots, n$). The function that assigns the edge $E_{j_ik_i}$ to the vertex P_i is called the Gromov product structure on X. Two Δ-generic metric spaces (X, d) and (X, d') are called Δ-equivalent, if the corresponding Gromov product structures are the same up to a permutation of X.

Δ-equivalence classes for 5-point metrics coincide with the hypersimplex decomposition [7,8], obtained from the metric fan [2]. The Δ-equivalence classes and hypersimplex decomposition of 6-point spaces were given, respectively, in [2] and [8]. The algorithm for Δ-equivalence class decompositions is based on the following Proposition 1 and Corollary 1 of [2].

Proposition 1. *Let (X, d) be a finite metric space with n elements P_i, $i = 1, \ldots, n$. Then the following equations hold*

$$\Delta_{ijl} - \Delta_{ijk} = \Delta_{kjl} - \Delta_{kil} = \Delta_{lik} - \Delta_{ljk} = \Delta_{jik} - \Delta_{jil},$$

where $i, j, k, l = 1, 2, \ldots, n$.

Corollary 1. *Let (X, d) be a Δ-generic finite metric space and let Δ_{ijk} be the minimal Gromov product at node P_i. Then,*

(a) Δ_{jkl} cannot be minimal at node P_j, where $l \neq j, k$
(b) Δ_{kjl} cannot be minimal at node P_k, where $l \neq j, k$
(c) Δ_{lij} and Δ_{lik} cannot be minimal at node P_l, where $l \neq i, j, k$

In order to obtain a decomposition of finite metric spaces into Δ-equivalence classes, we start by the Cartesian product of the sets of Gromov products at each P_i, then use Corollary 1 in order to eliminate the ones that are not allowable. Then, the permutation group on n elements is acted on the list of allowable Gromov products to form the orbits under this group action. A representative from each Δ-equivalence class is selected to form a list. We note that Corollary 1 gives necessary conditions in the sense that the list obtained may contain structures that may not be realizable as generic Δ-equivalence classes. These can be eliminated by using an algorithm based on combinatorial arguments, as presented in [6].

Gromov product structures on a (generic) n-point metric space have a convenient representation by an $n \times n$ matrix M_Δ defined by $M_\Delta(i, j) = 1$ and $M_\Delta(i, k) = 1$ if Δ_{ijk} is the minimal Gromov product at P_i and 0 otherwise [3]. Thus, a Δ-equivalence class corresponds to the orbit of the matrix representation M_Δ of a Gromov Product structure, under the action $P^{-1}M_\Delta P$ where P is the permutation matrix on the vertices of the space.

In Section 2, the hypersimplex classification is recalled and its relation to the Gromov product structures is clarified. In Section 3, a new classification tool in terms of 4-point subsets of a finite metric space called "Quadrangle Structure" is defined. In Section 4, metrics of type 12, 13, 39, 65 and 66 of the hypersimplex classification [8] are studied considering their Gromov product and quadrangle structures. We will present elsewhere that for $n = 5$, all three classification concepts give the same classes as in [7] and from $n = 6$ on, all three classification concepts begin to differ. In Section 5, split metric decompositions are reviewed and necessary and sufficient conditions for the isolation index of an m-split to be nonzero, in terms of quadrangle structures, are derived. In Section 6, the tools developed throughout the paper are used to construct a totally split decomposable metric on a 6-point space.

2. The metric Fan and Gromov product structures

In this section, we recall the definitions concerning the metric fan classification of finite metric spaces and relate the Gromov product structures to them.

The set C_n of all pseudo-metrics $d = (d_{ij}) \in \mathbb{R}^{\binom{n}{2}}$ on a given n-point set X, is called the metric cone (Since for a pseudo-metric, $d_{ij} = d_{ji}$, C_n can be thought as a subset of $\mathbb{R}^{\binom{n}{2}}$.) A decomposition of C_n into some sub-cones can be defined as follows [8].

Consider the $\binom{n}{2} \times n$ matrix $\mathcal{A}$ where the rows are labeled by

$$(1, 2), (1, 3), \ldots, (1, n), (2, 3), (2, 4), \ldots, (2, n), \ldots, (n - 1, n)$$

and the (i, j)-row $(i < j)$ is given by $e_i + e_j = (0, \ldots, 1, \ldots, 1, \ldots, 0) \in \mathbb{R}^n$.

Let $\mathcal{B}$ be an invertible $n \times n$ submatrix of $\mathcal{A}$ and denote the $\left[\binom{n}{2} - n\right] \times n$ matrix obtained by deleting $\mathcal{B}$ from $\mathcal{A}$ by $\mathcal{B}'$. Likewise, define $d_{\mathcal{B}} \in \mathbb{R}^n$ by choosing the components of $d \in \mathbb{R}^{\binom{n}{2}}$ corresponding to $\mathcal{B}$ and $d_{\mathcal{B}'} \in \mathbb{R}^{\binom{n}{2}-n}$ corresponding to $\mathcal{B}'$. Now consider the following system of equations and inequalities for $x \in \mathbb{R}^n$:

$$\mathcal{B}x = d_{\mathcal{B}} \ \text{ and } \ \mathcal{B}'x > d_{\mathcal{B}'}.$$

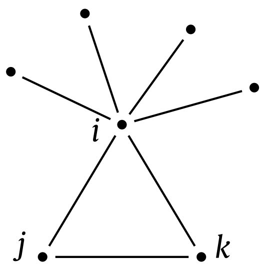
If this system has a solution we say that the matrix $\mathcal{B}$ is a "cell" or a "thrackle" for the metric d. We denote the collection of cells of a metric d by $Cell(d)$. This terminology stems from the fact that the row vectors of $\mathcal{B}$ can be viewed as the vertices of an $(n - 1)$-simplex in $\mathbb{R}^n$. Still another interpretation is that, a row vector $e_i + e_j$ can be viewed as an edge of the complete graph K_n with n nodes so that a cell $\mathcal{B}$ can be viewed as a sub-graph of K_n.

Now we define two metrics d and d' on an n-point set X to be equivalent if they have the same collection of cells, i.e. $Cell(d) = Cell(d')$ (or what amounts to the same, the same collection of sub-graphs). The equivalence class of a metric d is a sub-cone of the metric cone and these sub-cones constitute altogether the metric fan.

We will now give a characterization of Gromov product structure in terms of sub-graphs in the metric fan picture.

Proposition 2. *Let $(X = \{P_1, P_2, \ldots, P_n\}, d)$ be an n-point metric space. Then, (X, d) is Δ-generic with the Gromov product structure $P_i \mapsto E_{jk}, (i = 1, \ldots, n)$ if and only if the following sub-graphs $G_{i,jk}$ of (the complete graph) K_n belong to the cell-collection $Cell(d)$ of the metric d.*

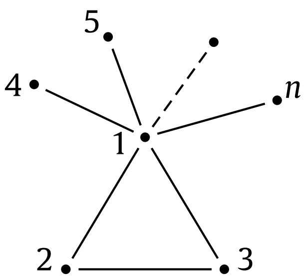
$G_{i,jk}$:



The unlabeled vertices have the labels from $\{1, 2, \ldots, n\} \setminus \{i, j, k\}$.

Proof. For the ease of notation let $i = 1,\ j = 2,\ k = 3$. Then, the graph $G_{1,23}$ corresponds to the matrix $\mathcal{B}$ below:

$G_{1,23}$:



$$\longleftrightarrow \qquad \mathcal{B} = \begin{bmatrix} 1 & 1 & 0 & \ldots & 0 \\ 1 & 0 & 1 & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & 0 & \ldots & 1 \\ 0 & 1 & 1 & \ldots & 0 \end{bmatrix}$$

The system $\mathcal{B}x = d_{\mathcal{B}}$ and $\mathcal{B}'x > d_{\mathcal{B}'}$ reads as follows:

$$\begin{array}{rclrcl} x_1 + x_2 & = & d_{12} & x_2 + x_4 & > & d_{24} \\ x_1 + x_3 & = & d_{13} & & \vdots & \\ x_1 + x_4 & = & d_{14} & x_2 + x_n & > & d_{2n} \\ & \vdots & & & \vdots & \\ x_1 + x_n & = & d_{1n} & x_r + x_s & > & d_{rs}\ \ (r \geq 2,\ s \geq 4,\ r < s) \\ x_2 + x_3 & = & d_{23} & & \vdots & \\ & & & x_{n-1} + x_n & > & d_{n-1\ n}. \end{array}$$

If the system has a solution in terms of x_i's, then Δ_{123} is uniquely minimal among Δ_{1rs} for $1 \neq r \neq s \neq 1$ and vice versa. To show this, first consider the first 2 equations and the last one from left column to see that $x_1 = \Delta_{123}$, $x_2 = \Delta_{213}$ and $x_3 = \Delta_{312}$. From other equations it follows that $x_k = d_{1k} - \Delta_{123}$ for $4 \leq k \leq n$. By applying algebraic manipulations, it can be seen that the inequalities $x_2 + x_k > d_{2k}$ $(4 \leq k \leq n)$ are equivalent to $\Delta_{123} < \Delta_{12k}$, the inequalities $x_3 + x_k > d_{3k}$ $(4 \leq k \leq n)$ are equivalent to $\Delta_{123} < \Delta_{13k}$ and finally the inequalities $x_r + x_s > d_{rs}$ $(4 \leq r, s$ and $r < s)$ are equivalent to $\Delta_{123} < \Delta_{1rs}$. Applying this to every node of X, the proposition follows. ■

This proposition shows that Gromov product equivalence is weaker than the metric fan equivalence:

Proposition 3. *Let d and d' be two Δ-generic metrics on an n-point set $X = \{P_1, P_2, \ldots, P_n\}$. If d and d' are equivalent in the metric fan sense, i.e. $Cell(d) = Cell(d')$, then they have the same Gromov product structure (and so, a fortiori, they are equivalent in the Gromov product sense).*

Proof. If the Δ-generic metric d has the Gromov product structure $P_i \to E_{jk}$, for $i = 1, 2, \ldots, n$, then by Proposition 2 the sub-graphs $G_{i,jk}$ of (the complete graph) K_n belong to the cell-collection $Cell(d)$ of the metric d. Since by assumption $Cell(d) = Cell(d')$, the sub-graphs $G_{i,jk}$ belong also to $Cell(d')$. This means, again by Proposition 2, that the metric d' has the same Gromov product structure. ■

3. Quadrangle structures

In this section we define a new kind of structure on a finite metric space.

Definition 3. An n-point finite metric space X is called "quadrangle generic", or Q-generic, if for every 4-point subset $\{P_i, P_j, P_k, P_l\} \subseteq X$, the set of distances

$$\{d_{ij} + d_{kl},\ d_{ik} + d_{jl}, d_{il} + d_{jk}\}$$

has a unique maximal element.

We remark that for a 4-point metric space the notions of Δ-genericness and Q-genericness coincide. Let $X = \{P_a, P_b, P_c, P_d\}$ be a 4-point metric space. If X is Δ-generic and if we assume without loss of generality that the minimal Gromov product at P_a is Δ_{abd}, then we have the relations

$$\Delta_{abc} - \Delta_{abd} = \tfrac{1}{2}(d_{ab} + d_{ac} - d_{bc}) - \tfrac{1}{2}(d_{ab} + d_{ad} - d_{bd}) = \tfrac{1}{2}(d_{ac} + d_{bd} - d_{ad} - d_{bc}) > 0$$
$$\Delta_{acd} - \Delta_{abd} = \tfrac{1}{2}(d_{ac} + d_{ad} - d_{cd}) - \tfrac{1}{2}(d_{ab} + d_{ad} - d_{bd}) = \tfrac{1}{2}(d_{ac} + d_{bd} - d_{ab} - d_{cd}) > 0,$$

which show that $d_{ac} + d_{bd}$ is the unique maximal element of the set $\{d_{ab} + d_{cd}, d_{ac} + d_{bd}, d_{ad} + d_{bc}\}$. Hence X is Q-generic. Conversely if $X = \{P_a, P_b, P_c, P_d\}$ is Q-generic with $d_{ac} + d_{bd}$ the maximal element of the set $\{d_{ab} + d_{cd}, d_{ac} + d_{bd}, d_{ad} + d_{bc}\}$, then X is Δ-generic with Δ_{abd} the minimal Gromov product at P_a. Likewise, Δ_{bac} is the minimal Gromov product at P_b, Δ_{cbd} at P_c and Δ_{dac} at P_d. Hence X is Δ-generic.

We now define the notion of a quadrangle structure:

Definition 4. A quadrangle structure on a Q-generic finite metric space (X, d) is a map which assigns to any 4-point subset $\{P_a, P_b, P_c, P_d\}$ of X the pair of edges corresponding to the maximal element of the set $\{d_{ab} + d_{cd}, d_{ac} + d_{bd}, d_{ad} + d_{bc}\}$.

If, for example, $d_{ac} + d_{bd}$ is the maximal element of the set $\{d_{ab} + d_{cd}, d_{ac} + d_{bd}, d_{ad} + d_{bc}\}$, then the pair $\{E_{ac}, E_{bd}\}$ is assigned to the 4-point subset $\{P_a, P_b, P_c, P_d\}$. We will say that the edges E_{ac} and E_{bd} are "diagonals" and the edges E_{ab}, E_{ad}, E_{bc}, E_{cd} are "sides".

We denote the 4-point subset $\{P_a, P_b, P_c, P_d\}$ without any restriction on the sides by $Q(a, b, c, d)$. In this notation the ordering of the indices is irrelevant. On the other hand, if $d_{ac} + d_{bd}$ is maximal, then the vertices should be ordered as (P_a, P_b, P_c, P_d) and we denote this structured quadrangle by $Q(abcd)$. Clearly, cyclic permutation and reversal of the order of the indices give equivalent quadrangles.

Definition 5. Two Q-generic finite metric spaces (X, d) and (X, d') are called Q-equivalent, if the corresponding quadrangle structures are same up to a permutation of X.

Although, quadrangle structures are defined independently of Gromov product structures, in what follows we prefer to work with quadrangle structures that are partially determined by a given Gromov product structure: If Δ_{ijk} is minimal at P_i, then for all 4-point subsets $\{P_i, P_j, P_k, P_l\}$, $d_{il} + d_{jk}$ is maximal. Thus, the Gromov product structure determines the structure of part of the quadrangles. Further discussions will be given in Section 4. It is worth to mention that for $n = 5$, the Gromov product structure determines the quadrangle structure completely.

The matrix representation for a quadrangle structure is defined as below.

Definition 6. The matrix M_Q of a quadrangle structure Q on an n-point metric space, is an $n_d \times n_d$ matrix ($n_d = n(n-1)/2$) such that $M_Q(ab, cd) = 1$ if the edges E_{ab} and E_{cd} are diagonals in $\{P_a, P_b, P_c, P_d\}$, and $M_Q(ab, cd) = 0$ otherwise.

Note that here again the rows and columns are labeled by $(1, 2), (1, 3), \dots, (1, n), (2, 3), (2, 4), \dots, (2, n), \dots, (n-1, n)$ and the rows and columns of this matrix related to the edges that are never diagonals in any of the quadrangles they occur, consist of zeros.

A Q-equivalence class thus corresponds to the orbit of the matrix representation M_Q of the quadrangle structure under the action $\tilde{P}^{-1} M_Q \tilde{P}$ where $\tilde{P}$ is the permutation matrix on the edges induced by the permutation of the vertices of the space.

4. The relation between Gromov product structures, quadrangle structures and the hypersimplex classification

In this section we illustrate the relations between Gromov product structures, quadrangle structures and the hypersimplex classification by an example.

Metrics that belong to the Δ-equivalence class I_{17}, introduced in [2] are characterized by the minimality of the Gromov products

$$\{\Delta_{126}, \Delta_{213}, \Delta_{324}, \Delta_{435}, \Delta_{546}, \Delta_{615}\}. \tag{3}$$

In [2], it was shown that the metrics numbered as 12, 13, 39, 65 and 66 in the hypersimplex classification [8] belong to this Δ-equivalence class, after relabeling of the vertices as

$$\begin{aligned} &(1, 2, 3, 4, 5, 6) \to (1, 2, 6, 4, 3, 5), \quad \text{for types } 12, 13 \\ &(1, 2, 3, 4, 5, 6) \to (1, 2, 6, 3, 5, 4), \quad \text{for types } 39, 65, 66. \end{aligned} \tag{4}$$

In order to determine the quadrangle structures of the metrics above one needs to find the maximal element of the sets $\{d_{ab} + d_{cd}, d_{ac} + d_{bd}, d_{ad} + d_{bc}\}$. For this aim, we use the Gromov product structure of class I_{17} to determine the quadrangle structure partially, which means to determine the structure of a part of the quadrangles using Gromov products.

For $n = 6$ there are 15 quadrangles. It can be seen that the structures of 12 of these quadrangles belonging to the metric class I_{17}, is determined by the minimality of Gromov products of this Δ-equivalence class. To make this clear, consider the quadrangle $Q(1, 2, 3, 4)$ for instance. For the class I_{17}, Δ_{213} is the unique minimal Gromov product at vertex 2, so $\Delta_{213} < \Delta_{214}$, or equivalently $\frac{1}{2}(d_{12} + d_{23} - d_{13}) < \frac{1}{2}(d_{12} + d_{24} - d_{14})$ or equivalently $d_{14} + d_{23} < d_{13} + d_{24}$. Similarly from $\Delta_{213} < \Delta_{234}$ one obtains that $d_{12} + d_{34} < d_{13} + d_{24}$. This means that for the quadrangle $Q(1, 2, 3, 4)$, E_{13} and E_{24} appear as diagonals and the structure of the quadrangle is determined as $Q(1234)$. This is in fact the way that we can determine the structure of a part of quadrangles by Gromov product structure. The fact that the structure of $Q(1234)$ could be determined by the minimality of Δ_{213} is depicted by an arc on the vertex 2 of $Q(1234)$ as shown in Fig. 1. The additional arc on vertex 3 of $Q(1234)$ means that this result could also be obtained by the minimality of Δ_{324}. For the class I_{17} these same calculations are done at each vertex and it happens that the structures of 12 quadrangles out of 15 are determined as shown in Fig. 1.

A priori, each of the quadrangles $Q(1, 2, 4, 5)$, $Q(1, 3, 4, 6)$ and $Q(2, 3, 5, 6)$ can have 3 structures; for example, for $Q(1, 2, 4, 5)$ diagonal pairs can be $\{E_{12}, E_{45}\}$, $\{E_{14}, E_{25}\}$ or $\{E_{15}, E_{24}\}$. But, by comparing inequalities among Gromov products, it is possible to see that the minimum of $\{\Delta_{124}, \Delta_{125}, \Delta_{145}\}$ is either Δ_{124} or Δ_{125}, but it cannot be Δ_{145}. To see this assume that Fig. 1 (without arcs) is given. The structure of $Q(1, 2, 3, 5)$ is given as $Q(1235)$ which implies $\Delta_{125} < \Delta_{135}$. Also the structure of $Q(1, 3, 4, 5)$ is given as $Q(1345)$ which implies $\Delta_{135} < \Delta_{145}$. Combining these two, results in $\Delta_{125} < \Delta_{145}$, which is to say that Δ_{145} cannot be the minimum hence $\{E_{12}, E_{45}\}$ is not a diagonal pair. It follows that the structure of the quadrangle $Q(1, 2, 4, 5)$ can be either $Q(1245)$ or $Q(1254)$. In the former case the ordering of the vertices is in agreement with the ordering of the vertices for the remaining quadrangles, hence we call $Q(1245)$ of type S, to sand for "straight" and in the latter case we call $Q(1254)$ of type T, to stand for "twisted".

By similar arguments it can be seen that the three quadrangles $Q(1, 2, 4, 5)$, $Q(1, 3, 4, 6)$ and $Q(2, 3, 5, 6)$ can be of types S or T, which amounts to a total of 8 choices. But it can be shown that the quadrangle structures SST, STS and TSS can be mapped to each other by a permutation of indices and the same holds for types STT, STS and TTS. On the other hand, computations on the matrix of the quadrangle structures shows that the types SSS, SST, STT and TTT are inequivalent. It

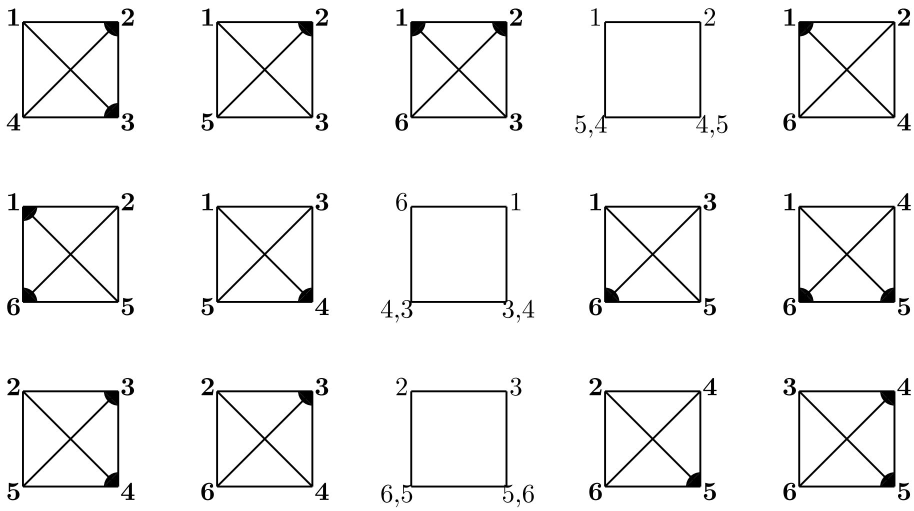


Fig. 1. The structure of the quadrangles of 6-point metric class I_{17} determined by its Gromov product structure.

follows that there are 4 distinct quadrangle types corresponding to a single Gromov product type.

$$\begin{aligned}
\text{Type}(SSS) &: Q(1245), Q(2356), Q(3461),\\
\text{Type}(SST) &: Q(1245), Q(2356), Q(3416),\\
\text{Type}(STT) &: Q(1245), Q(2365), Q(3416),\\
\text{Type}(TTT) &: Q(1254), Q(2365), Q(3416).
\end{aligned}$$

This example illustrates how the Gromov product structure partially determines the quadrangle structure of the given metric. It is worthwhile to mention that the reverse process is also important; selecting a diagonal for a quadrangle is to imply 8 relations between 12 Gromov products related to vertices of the underlying quadrangle. This means that the quadrangle structure can be used to obtain partial order relations among the Gromov products at each point. We should also note that, the metrics 12 and 13 of [8] both fall inside the structure which has all its 'free' quadrangles as twisted or TTT.

5. Split metric decompositions

A "split" $S = \{A, B\}$ of a finite set X is a partition of X into two non-empty subsets A and B. For simplicity we often identify the set of points of A with its index set. For each $P_a \in X$, we denote by $S(a)$ the subset A or B that contains P_a. Corresponding to each split S we define the pseudo-metric δ_S by

$$\delta_S(a, a') = \begin{cases} 1 & \text{if } S(a) \neq S(a'), \\ 0 & \text{if } S(a) = S(a'). \end{cases}$$

This pseudo-metric on X is called a split-metric or cut-metric on X [4]. As the split $S = \{A, B\}$ of the set X is already determined by A, this split metric is also denoted by δ_A. If $A \subset X$ has k elements, the split $\{A, B\}$ is called a k-split (or equivalently, an $(n - k)$-split). When $A = \{P_a\}$ or $\{P_a, P_b\}$ the corresponding 1-split and 2-split are simply denoted by δ_a and δ_{ab} respectively.

A metric on X is called totally split decomposable if it can be expressed as a linear combination (with non-negative coefficients) of the split metrics [1].

The isolation index of a split $S = \{A, B\}$ is defined as

$$\alpha_{A,B} = \frac{1}{2} min_{a,a' \in A, b,b' \in B}\{max\{d_{ab} + d_{a'b'}, d_{ab'} + d_{a'b}, d_{aa'} + d_{bb'}\} - (d_{aa'} + d_{bb'})\}.$$

Proposition 4. *Let (X, d) be a finite metric space with n elements P_i $(i = 1, \ldots, n)$ and let $S = \{A, B\}$ be a split decomposition for X. Then,*

i. The isolation index for the 1-split with $A = \{P_a\}$ is the minimal Gromov product at P_a,
ii. If (X, d) is Q-generic, then the isolation index for the k-split with $A = \{P_{i_1}, \ldots, P_{i_k}\}$ is non-zero if and only if for no pair of indices $a, a' \in A$, $E_{aa'}$ is a diagonal of the quadrangles $Q(a, a', b, b')$ where $b, b' \in B$.

Proof. **i.** If $A = \{P_a\}$ and $B = \{P_{b_1}, \ldots, P_{b_{n-1}}\}$, then since $a = a'$, $d_{aa'} = 0$, the expression of the isolation index is

$$\alpha_{\{P_a\},B} = \frac{1}{2} min_{b,b' \in B} \{max\{d_{ab} + d_{ab'}, d_{ab'} + d_{ab}, d_{bb'}\} - d_{bb'}\}$$
$$= \frac{1}{2} min_{b,b' \in B} \{max\{d_{ab} + d_{ab'}, d_{bb'}\} - d_{bb'}\}.$$

By triangle inequality, $d_{ab} + d_{ab'} \geq d_{bb'}$, thus

$$\alpha_{\{P_a\},B} = \frac{1}{2} min_{b,b' \in B} \{d_{ab} + d_{ab'} - d_{bb'}\}. \tag{5}$$

This means that the isolation index for the case $A = \{P_a\}$ is the minimal Gromov product at P_a.

ii. Let us now compute the isolation index for the case where A is a 2-point set $\{P_a, P_{a'}\}$, or by our abuse of notation $\{a, a'\}$. By definition

$$\alpha_{\{a,a'\},B} = \frac{1}{2} min_{b,b' \in B} \{max\{d_{ab} + d_{a'b'}, d_{ab'} + d_{a'b}, d_{aa'} + d_{bb'}\} - (d_{aa'} + d_{bb'})\}$$

If $E_{aa'}$ is a diagonal in at least one quadrangle $Q(a, a', b, b')$, then $d_{aa'} + d_{bb'}$ is maximal among $\{d_{ab} + d_{a'b'}, d_{ab'} + d_{a'b}, d_{aa'} + d_{bb'}\}$ and thus the isolation index $\alpha_{\{a,a'\},B}$ vanishes. If, on the other hand, $E_{aa'}$ is a side in every quadrangle $Q(a, a', b, b')$ for $b, b' \in B$, then $d_{aa'} + d_{bb'}$ is strictly less than $max\{d_{ab} + d_{a'b'}, d_{ab'} + d_{a'b}, d_{aa'} + d_{bb'}\}$ for all $b, b' \in B$ and consequently the isolation index $\alpha_{\{a,a'\},B}$ is strictly positive.

If A has more than 2 elements, the proof is essentially the same. ∎

6. Totally split decomposable metrics for $n = 6$

In this section we will make use of the concepts developed so far, specially quadrangle structure, to construct a totally split decomposable metric for $n = 6$. Let us consider 6-point metrics that are Δ and Q-generic. We recall that there are always 6 1-splits whose isolation indices are the minimal Gromov products. We will look for 6-point metrics that have 15 splits or equivalently a total of 9 2-splits or 3-splits. According to Corollary 5 of [1] any such metric is totally split decomposable. We first show that the number of 2-splits is at most 6 in any split decomposition. For this we need to define 2-split chains and cycles.

Definition 7. A 2-split chain of length k is a collection of edges

$$\{E_{a_1a_2}, E_{a_2a_3}, \ldots, E_{a_{j-1}a_j}, E_{a_ja_{j+1}}, \ldots, E_{a_ka_{k+1}}\}$$

such that the isolation indices of the corresponding 2-splits are nonzero. If $a_{k+1} = a_1$, then we say that there is a 2-split cycle of length k.

Lemma 1. *In a finite Δ and Q-generic metric space (X, d) with n elements, the number of 2-splits is at most n.*

Proof. To show this consider the subgraph X_{2s} of the complete graph X consisting of the edges E_{ij} which represent the 2-splits with the belonging vertices included. We claim that the vertices of X_{2s} have degree of at most 2. To show this, assume that the vertex i has a degree of more than 2, hence we can select the edges E_{ij}, E_{ik} and E_{il} from X_{2s}. Since these edges represent the 2-splits, by Proposition 3, these edges are sides in every quadrangle that they appear in, specially $Q(i, j, k, l)$. But this cannot happen because if any two of them are sides in the quadrangle $Q(i, j, k, l)$ the third cannot be anymore. Thus the subgraph X_{2s}, is a disjoint union of some paths and cycles (which we call the maximal split chains and cycles). Now, any vertex of X belongs to at most one of these components and the number of edges of the subgraph X_{2s}, that is the number of 2-splits, is no more than the number of vertices of X_{2s}, and thus at most n. ∎

By Lemma 1, for $n = 6$ there can be at most 6 2-splits and thus to use Corollary 5 of [1] we must have some 3-splits. To build up a totally split decomposable metric, first we start by selecting the 3-splits. For $n = 6$ there is a total of 10 3-splits. Assume that (A, A^c) is a 3-split, where A is a 3 point set. For any other 3-split (B, B^c), if A and B have empty intersection, then B is the complement of A. Furthermore, if A and B have 1 element in common, then A and the complement of B will have 2 elements in common, therefore we may assume that, for $n = 6$ any system of 3-splits contains

$$\delta_A = (\{P_1, P_2, P_3\}, \{P_4, P_5, P_6\}), \qquad \delta_B = (\{P_1, P_2, P_6\}, \{P_3, P_4, P_5\}).$$

(For simplicity we will refer to a split $\delta_A = (A, A^c)$ as A.)

Recall that if δ_A, where $A = \{P_a, P_b, P_c\}$, is a 3-split then by Proposition 3, E_{ab} is a side in every quadrangle that does not contain P_c as a vertex, likewise for E_{ac} and E_{bc} and the structure of the quadrangles that contain all three points P_a, P_b and P_c is not determined. Using this and going through all 15 quadrangles, it can be seen that the structure of the quadrangles $Q(1, 3, 4, 6)$, $Q(1, 3, 5, 6)$, $Q(2, 3, 4, 6)$, $Q(2, 3, 5, 6)$ are completely determined as shown in Fig. 2 as $Q(1346)$, $Q(1356)$, $Q(2346)$, $Q(2356)$.

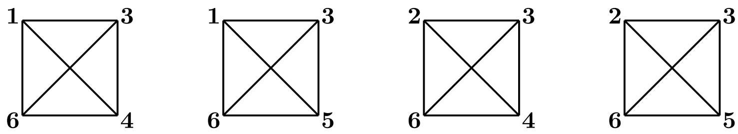


Fig. 2. The structures of the quadrangles $Q(1346)$, $Q(1356)$, $Q(2346)$, $Q(2356)$.

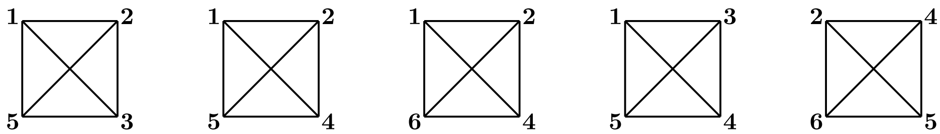


Fig. 3. The structures of the quadrangles $Q(1235)$, $Q(1245)$, $Q(1246)$, $Q(1345)$, $Q(2456)$.

To add a third 3-split to this list, first we note that in the quadrangle $Q(1346)$, E_{14} and E_{36} are diagonals, hence the 3-split $\{P_1, P_2, P_4\}$ cannot be added, otherwise it would violate Proposition 3. Similarly, in the quadrangle $Q(1356)$, E_{15} and E_{36} are diagonals, hence the splits $\{P_1, P_2, P_5\}$ and $\{P_1, P_4, P_5\}$ are eliminated. Likewise, in the quadrangle $Q(2346)$, E_{24} and E_{36} are diagonals, hence $\{P_1, P_3, P_6\}$ is eliminated. The quadrangle $Q(2356)$ is not helpful in eliminating more 3-splits from the list of 10 3-splits for a 6-point space.

It follows that the list of remaining allowable 3-splits is reduced to

$$\{P_1, P_3, P_4\}, \ \{P_1, P_3, P_5\}, \ \{P_1, P_4, P_6\}, \ \{P_1, P_5, P_6\}.$$

Since the 3-splits above are invariant under the interchange of (P_4, P_5), as the third 3-split of the system, one can choose either $\{P_1, P_5, P_6\}$ or $\{P_1, P_3, P_5\}$. Both of these choices lead to a system of 3-splits of the form $\{P_1, P_2, P_3\}, \ \{P_1, P_2, P_6\}, \ \{P_1, P_5, P_6\}$, or $\{P_1, P_2, P_3\}, \ \{P_1, P_2, P_6\}, \ \{P_1, P_3, P_5\}$, respectively. Therefore one can choose the system of 3-splits

$$A = \{P_1, P_2, P_3\}, \qquad B = \{P_1, P_2, P_6\}, \qquad C = \{P_1, P_5, P_6\}.$$

Among the quadrangles, this third split C, when Proposition 3 is considered again, determines the structure of 5 more quadrangles as depicted in Fig. 3.

Now that the structure of 9 quadrangles are fully determined and for the quadrangles $Q(1, 2, 3, 4)$, $Q(1, 2, 3, 6)$, $Q(1, 2, 5, 6)$, $Q(1, 4, 5, 6)$, $Q(2, 3, 4, 5)$, $Q(3, 4, 5, 6)$ the edges $E_{34}, E_{16}, E_{12}, E_{45}, E_{23}, E_{56}$ are sides, we can follow two paths: first is to add the fourth 3-split $\{P_1, P_3, P_5\}$, which in this case one can see that the structure of all of the quadrangles will be determined and addition of any 2-split will violate Proposition 3. In fact this case (sum of 4 3-splits) is the metric 339 of [8]. Second, instead of adding a fourth 3-split, one can see that without violating Proposition 3, 6 2-splits

$$\{P_1, P_2\}, \ \{P_1, P_6\}, \ \{P_2, P_3\}, \ \{P_3, P_4\}, \ \{P_4, P_5\}, \ \{P_5, P_6\}.$$

can be added to the 3-splits discussed above which in turn determine the structure of all 15 quadrangles. This second case (sum of 6 2-splits plus sum of 3 3-splits) according to Corollary 5 of [1], is a totally split decomposable metric which is in fact the 6-point metric type 66 of [8]. According to [8] this is the only totally split decomposable metric for $n = 6$.

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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