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On the Properties of Gromov Matrices and Their Applications in Network Inference

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Abstract

The spanning tree heuristic is a commonly adopted procedure in network inference and estimation. It allows one to generalize an inference method developed for trees, which is usually based on a statistically rigorous approach, to a heuristic procedure for general graphs by (usually randomly) choosing a spanning tree in the graph to apply the approach developed for trees. However, there are an intractable number of spanning trees in a dense graph. In this paper, we represent a weighted tree with a matrix, which we call a Gromov matrix. We propose a method that constructs a family of Gromov matrices using convex combinations, which can be used for inference and estimation instead of a randomly selected spanning tree. This procedure increases the size of the candidate set and hence enhances the performance of the classical spanning tree heuristic. On the other hand, our new scheme is based on simple algebraic constructions using matrices, and hence is still computationally tractable. We discuss some applications on network inference and estimation to demonstrate the usefulness of the proposed method.

I. INTRODUCTION

Information is being propagated across networks like online social networks with increasing speed due to better connectivity. There has been recent increased interest in inference and estimation problems on networks. For example, information dynamics and social learning have been investigated in [1], [2], [2]–[8]. Finding the sources of an infection or rumor diffusing in a network has been investigated in various works, including [9]–[16]. Networks are usually modeled mathematically using graphs. Many research works (for example, [9], [10], [16]) on network inference adopts the following strategy:

- (i) One first establishes theoretical results on tree networks. In many practical applications, it is reasonable to assume that information propagation follows a spanning tree. Furthermore, the uniqueness of a simple path between any pair of nodes greatly simplifies the theoretical analysis, making it tractable to obtain theoretically rigorous results.

- (ii) A tree-based algorithm or estimator is proposed based on the theoretical studies on trees.
- (iii) The algorithm or estimator is extended to general graphs using the spanning tree heuristic: a spanning tree of a selected set of nodes is found. The tree-based algorithm or estimator in (ii) is then applied to this tree. An additional optimization procedure may be used to arrive at the final estimate for the general graph.

An example is given as follows.

Example 1. *Consider the network infection source estimation problem in which an infection starting from a source node propagates along the edges of a graph $G = (V, E)$. A snapshot $I \subset V$ of all the infected nodes is observed, and we wish to estimate the identity of the source node (see for example [9], [16], [17]). One possible approach is to minimize a real-valued estimator function $e(s, T)$ over each candidate source node $s \in V$, and each breadth-first search (BFS) tree T rooted at s , which spans the infected nodes I . To make this optimization procedure computationally tractable for a general graph, for each candidate source node s , a random BFS tree T_s is usually chosen (e.g., [9], [16], [17]), and the source node is estimated by $\arg \min_{s \in V} e(s, T_s)$.*

The idea behind this approach is that for each realization of the infection process, the infected set I is spanned by a BFS tree rooted at the true source node. The BFS tree is unknown a priori. By randomly choosing a BFS tree for each s , even if s happens to be the true source node, it is unlikely that the chosen BFS tree is the actual infection tree if G is a dense graph. An arguably better approach is to find $\min_{s, T \in \mathcal{T}_s} e(s, T)$, where $\mathcal{T}_s$ is a family of BFS trees rooted at s that span I , which is restricted to be small enough so that the minimization procedure is computationally tractable.

There are other variants of this problem. For example, instead of observing a snapshot status of all the nodes of G , one may observe the infection timestamps of a small portion of the network. The source is estimated using such timestamp information (e.g., [10], [18]–[20]). Similar heuristics involving BFS trees have also been proposed.

The family of trees $\mathcal{T}_s$ rooted at s in Example 1 needs to be chosen carefully. For example, in the extreme case, Cayley’s formula states that the number of spanning trees in a complete graph with n vertices is n^{n-2} . In this paper, our aim is to propose an approach to construct a reasonable $\mathcal{T}_s$ to partially overcome such an intractability problem. We propose the use of Gromov matrices (which we define in Section II) to represent a weighted tree in a graph. Then

by taking appropriate convex combinations of a small set of such Gromov matrices, we can generate a tractable convex set $\mathcal{T}_s$ over which our estimator function can be optimized.

This paper takes its root in [20], in which we introduced the use of a Gromov matrix to represent an *unweighted* tree. In this paper, we further refine and generalize our Gromov matrix approach to weighted graphs, prove various properties of the Gromov matrices and demonstrate how to apply Gromov matrices in several network inference problems. A preliminary version of this paper was published in the conference [21].

The rest of the paper is organized as follows. In Section II, we introduce the notion of a Gromov matrix and its properties. In Section III, we demonstrate geometrically how a tree is constructed from a single point by a series of simple steps. The discussions lead to an iterative way to construct a Gromov matrix, and provides tools to investigate various properties of such matrices. In Section IV, we explain how to construct a parametric family of trees from a fixed finite set of trees using Gromov matrices. We discuss properties of this construction. We give applications of our method on network inference and estimation in Section V, and conclude in Section VI. Miscellaneous discussions and technical proofs of some results are given in the appendices.

Notations: Given a matrix M , we use $M(i, j)$ to denote its (i, j) -th entry. We write M^{-1} for its inverse. For a real symmetric matrix M , we denote its smallest eigenvalue by $\lambda_{\min}(M)$. For two nodes u and v in a tree, we use $[u, v]$ to denote the path from u to v and $(u, v]$ to denote the path with the end node u excluded. Other notations like $[u, v)$ and (u, v) are defined similarly. For a graph G , let $d_G(u, v)$ be the sum of the edge weights of the shortest path P in G between vertices u and v . The length of P is $d_G(u, v)$.

II. GROMOV MATRICES OF WEIGHTED TREES AND THE THREE-POINT CONDITION

Suppose that T is a weighted, undirected tree. The weight of each edge (u, v) is a positive real number.

Definition 1. Let s in T be a fixed node. For u, v in T , their Gromov product (see Definition 2.6 of [22]) with respect to (w.r.t.) s is defined as

$$(u, v)_s = \frac{1}{2}(d_T(u, s) + d_T(v, s) - d_T(u, v)). \quad (1)$$

For an ordered set of vertices $V = \{v_1, \dots, v_n\} \subset T$ that does not contain s , the associated Gromov matrix M is the matrix with (i, j) -th entry $M(i, j) = (v_i, v_j)_s$. We say that M has base (T, s, V) , where T is known as its base tree, s its base vertex, and V its base set.

We view a weighted tree as a metric space. Two weighted trees T_1 and T_2 are said to be *isometric* to each other if there is a bijection $\varphi : T_1 \rightarrow T_2$ such that $d_{T_1}(u, v) = d_{T_2}(\varphi(u), \varphi(v))$ for any $u, v \in T_1$. The map φ is called an isometry. We say that two bases (T_1, s_1, V_1) and (T_2, s_2, V_2) are *isometrically equivalent* to each other if there is an isometry $\varphi : T_1 \rightarrow T_2$ such that $\varphi(s_1) = s_2$ and $\varphi(V_1) = V_2$.

Suppose for a base (T, s, V) , T spans $V \cup \{s\}$. Proposition 1 of [20] may be generalized (using a similar proof) as follows: for each Gromov matrix, its base is uniquely determined, up to isometric equivalence. This observation tells us that the Gromov matrix contains all the information we want to describe a base.

In Corollary 2 in the sequel, we show that the Gromov matrix M is positive definite and symmetric. Conversely, not all positive definite symmetric matrices are Gromov matrices of a (weighted) tree as above, even if we assume the entries are non-negative numbers. Simple examples include:

$$\begin{bmatrix} 1 & 3 \\ 3 & 10 \end{bmatrix},$$

where the top-left diagonal entry 1 is smaller than the off-diagonals; and

$$\begin{bmatrix} 3 & 2 & 1 \\ 2 & 3 & 2 \\ 1 & 2 & 3 \end{bmatrix},$$

where the top-right and bottom-left entries are too small. We give below a condition that guarantees a matrix being the Gromov matrix of a weighted tree.

Definition 2. Let M be an $n \times n$ matrix. We say that M satisfies the three-point condition if the following holds: for any distinct indices i, j, k and any permutation x, y, z of $\{M(i, j), M(i, k), M(k, j)\}$, we have $x \geq \min\{y, z\}$ and equality holds if $y \neq z$.

For convenience, the triple x, y, z are called corners of the same rectangle (see Figure 1).

Fig. 1. Illustration of the notion of corners.

The three-point condition¹ requires that $\min\{x, y, z\}$ must occur at least twice among $\{x, y, z\}$.

Theorem 1. *An $n \times n$ symmetric matrix M is the Gromov matrix of a weighted tree if and only if the following conditions hold for M :*

- (a) *M has non-negative entries and all the diagonal entries of M are positive.*
- (b) *For all $1 \leq i, j \leq n$, $M(i, i) \geq M(i, j)$.*
- (c) *M satisfies the three-point condition.*

Proof: Suppose that M is a Gromov matrix with base (T, s, V) . It is easy to show that conditions (a) and (b) hold from Definition 2. To verify condition (c), suppose that $v_i, v_j, v_k \in V$ correspond to the distinct indices i, j, k of the matrix M . The branch point $p_{i,j}$ is defined as the unique vertex of T such that $[s, p_{i,j}] = [s, v_i] \cap [s, v_j]$. The branch points $p_{i,k}$ and $p_{k,j}$ are defined similarly. If $M(i, k) > M(k, j)$, then $p_{k,j} \in [s, p_{i,k}]$. Hence, we must have $p_{i,j} = p_{k,j}$ and $M(i, j) = M(k, j)$. The case $M(i, k) < M(k, j)$ is similar. If $M(i, k) = M(k, j)$, then $p_{i,k} = p_{k,j} \in [s, p_{i,j}]$. Hence $M(i, j) \geq M(i, k) = M(k, j)$. A similar argument holds for the two inequalities $M(i, k) \geq \min\{M(i, j), M(k, j)\}$ and $M(k, j) \geq \min\{M(i, k), M(i, j)\}$.

We prove the converse by induction on n . The case $n = 0, 1, 2$ are clearly true. Suppose the converse holds for all $k \times k$ symmetric matrices satisfying the conditions (a) – (c) and for all $k < n$. Consider a $n \times n$ symmetric matrix M satisfying conditions (a) – (c). By the induction hypothesis, we can construct a base (T', s, V') associated with the top-left $(n - 1) \times (n - 1)$

¹The name is due to its resemblance to the four-point condition in the theory of δ -hyperbolic metric space (cf. remark after Proposition 6.13 of [23]). In our case, the base s is fixed, therefore we only have to concern about the three remaining points.

matrix of M . We add an additional node v_n to V' as follows: Let $1 \leq j \leq n-1$ be the index such that $M(j, n) = \max\{M(i, n) : 1 \leq i \leq n-1\}$ with corresponding vertex $v_j \in V'$. Let p be the vertex on the path $[s, v_j]$ such that $d_{T'}(s, p) = M(j, n)$; and if it does not exist, we just let introduce it as a new vertex. We add an edge (v_n, p) of weight $M(n, n) - M(j, n) > 0$ to T' at p and set $T = T' \cup \{v_n\}$ and $V = V' \cup \{v_n\}$. The tree T is a well-defined weighted tree due to condition (b). Furthermore, $M(j, n) = (v_j, v_n)_s$ by construction.

To see that (T, s, V) is a base of M , consider any index $i \neq j$ such that $1 \leq i < n$ with corresponding vertex v_i . From the induction hypothesis, it suffices to show that $M(i, n) = (v_i, v_n)_s$ in T . We consider two cases below (see Fig. 2 for illustrations).

Suppose that $M(i, n) < M(j, n)$. Then, from the three-point condition (c), we have $M(i, j) = M(i, n)$. By our construction of p , the branch point $p_{i,n}$ is on the path $[s, p]$. This implies that $(v_i, v_n)_s = (v_i, v_j)_s = M(i, j) = M(i, n)$, where the penultimate equality is due to the induction hypothesis.

On the other hand, if $M(i, n) = M(j, n)$, then from the three-point condition (c), we have $M(i, n) = M(j, n) \leq M(i, j)$. Therefore, in our construction of p , we have $p \in [s, p_{i,j}]$ and $(v_i, v_n)_s = (v_j, v_n)_s = M(j, n) = M(i, n)$, where the penultimate equality is due to our construction. The converse is now proved, and so is the theorem. $\blacksquare$

Fig. 2. Illustration of the proof of Theorem 1.

We have the following immediate corollary regarding convex combinations of special Gromov matrices (see Fig. 3 for an example).

Corollary 1. *Suppose that M_1 and M_2 are Gromov matrices of weighted trees and M_2 is diagonal. Then for any $\theta \in [0, 1]$, the convex combination $M = \theta M_1 + (1 - \theta)M_2$ is the Gromov matrix of a weighted tree.*

Proof: It is easy to verify that M satisfies the three conditions of Theorem 1. ■

The conclusion does not hold in general if both M_1 and M_2 are not diagonal. In Section IV we describe a procedure to modify the convex combination of multiple Gromov matrices to a Gromov matrix.

Fig. 3. Let G be the graph in (a) and $V = \{v_1, v_2\}$. Consider three spanning trees T, T_1, T_2 of V and the base vertex s , as shown in (b), (c) and (d) respectively. Suppose M_T, M_{T_1} and M_{T_2} are the corresponding associated Gromov matrices. Then $M_T = 1/3 M_{T_1} + 2/3 M_{T_2}$.

III. ITERATIVE CONSTRUCTION OF A GROMOV MATRIX AND SOME SPECTRAL PROPERTIES

In this section, we show positive definiteness of the Gromov matrix M of a weighted tree T as a byproduct of finding a lower bound of its least singular value, i.e., the smallest eigenvalue of M . To do so, we describe an iterative way to construct M from the empty matrix (of size 0); and each step in the algebraic construction has a corresponding geometric counterpart, revealing additional geometric properties of T . We delegate some long technical proofs to the appendices.

For two square matrices M and N of sizes k and l respectively, we introduce the following operations, called the *Gromovication operations* for convenience:

- (a) Initialization: for $a > 0$, replace the empty matrix M by the 1×1 -matrix $M = (a)$.

- (b) Direct sum: $M \oplus N$ is the $(k + l) \times (k + l)$ square matrix with M and N forming the diagonal blocks; and 0 elsewhere.
- (c) Extension I (of M): for an integer $a > 0$, $\phi_a(M)$ is the $k \times k$ matrix obtained from M by adding a to each entry.
- (d) Extension II (of M): for two positive integers a, b such that $a \geq b > 0$, $\phi_{a,b}(M)$ is the $(k + 1) \times (k + 1)$ matrix obtained from M by adding a to each entry of M , followed by increasing the number of rows and columns of M each by one, and setting b as the entries of the $(k + 1)$ -th row and column.

Proposition 1. *M is the Gromov matrix of a weighted tree with vertex set $V \neq \emptyset$ if and only if for some permutation matrix P , $M' = PMP^{-1}$ can be obtained from the empty matrix by a finite sequence of Gromovication operations, starting with an initialization step.*

Proof: See Appendix A. ■

Suppose that M is a Gromov matrix. We study the its least singular value, which is defined as $\lambda_{\min}(M)$, the minimal eigenvalue of M . As a corollary, we prove that M is always positive definite.

Proposition 2. *Let M and N be Gromov matrices. We have the following results regarding the Gromovication operations.*

(a) *Direct sum:*

$$\lambda_{\min}(M \oplus N) = \min\{\lambda_{\min}(M), \lambda_{\min}(N)\}.$$

(b) *Extension I: For any positive integer a ,*

$$\lambda_{\min}(\phi_a(M)) \geq \lambda_{\min}(M).$$

(c) *Extension II: For any integers $a \geq b > 0$,*

(a) *If $a > b$,*

$$\lambda_{\min}(\phi_{a,b}(M)) \geq \min\{\lambda_{\min}(M), b - b^2/a\}.$$

(b) *If $a = b$,*

$$\lambda_{\min}(\phi_{a,a}(M)) \geq \frac{\lambda_{\min}(M)}{n + 1 + \lambda_{\min}(M)/a},$$

Fig. 4. Suppose M is a Gromov matrix with base (T, s, V) , where T is shown in the figure, V consists of the three red vertices; and s is the green vertex. Using our lower bound for direct sum and extension II, we see immediately that $\lambda_{\min}(M_T) \geq \min\{\min\{3, 3\}, 2 - 2^2/5\} = 1.2$. One can also compute that the eigenvalues (in increasing order) of M are 13.69, 3, 1.315; and the lower bound 1.2 is quite close in this case.

where n is the number of rows of M .

Proof: See Appendix B. ■

Proposition 2 can be useful in computation as shown in the example given in Fig. 4. Another immediate consequence is the following result.

Corollary 2. *Suppose that M is a Gromov matrix with base (T, s, V) . If V is non-empty, then M is positive definite.*

Proof: From Proposition 1, there exists a permutation matrix P such that $M' = PMP^{-1}$ is formed by a finite sequence of Gromovication operations. Note that M and M' have the same eigenvalues, thus it suffices to show that M' is positive definite. Since V is non-empty, we start with an initialization, making the matrix positive definite. From Proposition 2, the matrix M remains positive definite for any additional Gromovication operations, and the corollary is proven. ■

Intuitively, the least singular value of a Gromov matrix M encodes geometric information of its base tree T . If the least singular value of M is small, the leaves of T tend to be less branched off. We illustrate this intuition by a simple example in Fig. 5.

Fig. 5. In the three trees T_1, T_2, T_3 , it is easy to compute that the least singular value of the associated Gromov matrices $M_{T_1}, M_{T_2}, M_{T_3}$ (w.r.t. s and $\{v_1, v_2\}$) are $3, 2, 3 - \sqrt{5}$, respectively. Geometrically, T_3 is least branched off, while T_1 is most branched off.

IV. CONVEX COMBINATIONS OF GROMOV MATRICES

In this section, we discuss two different ways to construct new matrices from existing Gromov matrices based on convex combination. We also compare the advantages of each approach. Through a case study, we provide further insights into how well convex combinations of Gromov matrices can approximate an information propagation path in a network.

A. Two Types of Convex Combinations

Suppose we are given a finite collection of $n \times n$ Gromov matrices $\mathbf{M} = \{M_1, \dots, M_k\}$, all of the same dimensions. For each k -tuple of numbers $\alpha = (\alpha_1, \dots, \alpha_k) \in [0, 1]^k$ such that $\sum_{i=1}^k \alpha_i = 1$, define a new matrix as $M_\alpha = \sum_{i=1}^k \alpha_i M_i$. We call M_α the *convex combination* of $\mathbf{M}$, for convenience.

In general, the convex combination M_α is not always a Gromov matrix of any weighted tree, as the three-point condition is not preserved under matrix addition. There are various ways to modify the entries of M_α to obtain a Gromov matrix. We provide one such procedure here.

First set $M'_\alpha = M_\alpha$. Let $\mathbf{U}(M'_\alpha) = (x_1, \dots, x_{n(n-1)/2})$ denote the sequence of entries $M'_\alpha(i, j)$ with $i < j$ (i.e., the upper-triangular block excluding the diagonal) in non-increasing order with $x_1 \geq \dots \geq x_{n(n-1)/2}$. If x_t corresponds to $M_\alpha(i, j)$, then (i, j) is called the matrix indices of x_t . For each $t = 1, \dots, n(n-2)/2$ in increasing order, we perform the following steps:

(a) Search for every pair (x_u, x_v) satisfying the following two conditions:

- $u < t < v$; and
- x_u, x_t, x_v are corners of the same rectangle (Definition 2).

(b) If the matrix indices of x_v is (i, j) , we perform the following two steps:

- Set $x_v = x_t$ and $M'_\alpha(i, j) = x_t$.
- Move x_v to be immediately after x_t in $\mathbf{U}(M'_\alpha)$.

In doing so, the matrix indices of x_{t+1} becomes (i, j) and the sequence $\mathbf{U}(M'_\alpha)$ remains non-increasing.

Once the above procedure is completed, we symmetrize M'_α by assigning $M'_\alpha(i, j) = M'_\alpha(j, i)$ for all $i > j$. We call M'_α a *Gromovied convex (G-convex) combination* of $\mathbf{M}$ w.r.t. α . Note that for each t , there are at most n pairs (x_u, x_v) satisfying condition (a). The computational complexity of forming M_α is $O(kn^2)$. Therefore, the complexity of forming a G-convex combination M'_α is $O(kn^2 + n^3)$.

As we are enforcing the three-point condition each time we make an adjustment, the matrix M'_α is the Gromov matrix of a weighted tree by Theorem 1. The matrix M'_α has the property that $M'_\alpha(i, j) \geq M_\alpha(i, j)$ for any $1 \leq i, j \leq n$. Moreover, if M_α is already a Gromov matrix, then M'_α is the same as M_α .

Throughout the rest of this paper, when we talk about the convex or G-convex combination of a set of Gromov matrices $\mathbf{M}$, we assume for convenience that every Gromov matrix in $\mathbf{M}$ has the same base vertex and base set.

Let $G = (V_G, E)$ be a general graph, $U = \{u_1, \dots, u_n\} \subset V_G$ be a fixed set of distinct vertices of G and $s \in V_G$ a fixed node. In general, the spanning trees of U rooted at s are not unique and it is intractable to find all of them. However, if we are able to find a finite subset of spanning trees, we are able to use the G-convex combination construction to form a large family of trees $\mathcal{F}_s$. Doing so, we obtain a much larger candidate set than a randomly selected spanning tree, partially overcoming the intractability problem mentioned above. This can be useful in dealing with certain inference and estimation problems on graphs (see Section V). Note however that although each G-convex combination has a corresponding tree, this tree need not be a subgraph of G . On the other hand, we hope that $\mathcal{F}_s$ captures some distinctive structural features of s in G . We provide one such feature as follows.

Definition 3. Let T be a tree in a graph G spanning a subset of distinct vertices $U = \{u_1, u_2, u_3\}$ and a fixed base vertex $s \notin U$. The type of U in T is a partition of $U = U_1 \cup U_2$ such that $U_1 = \{u_i, u_j\}$ and $U_2 = \{u_l\}$ (where (i, j, l) is a permutation of the indices 1, 2, 3) and $(u_i, u_l)_s = (u_j, u_l)_s \leq (u_i, u_j)_s$.

Some thought will convince the reader that Definition 3 is non-vacuous and the type of any set of three distinct vertices exists. Furthermore, the type of $U = \{u_1, u_2, u_3\}$ is not unique if and only if $(u_1, u_2)_s = (u_1, u_3)_s = (u_2, u_3)_s$. Intuitively, the notion of type describes the relative positions of nodes in a tree w.r.t. a fixed base node. We provide Example 2 below to illustrate this notion. Before that, we first prove an elementary result.

Suppose we form the convex combination $M_\alpha = \theta M_1 + (1 - \theta)M_2$, where $\alpha = (\theta, 1 - \theta)$ and $\theta \in [0, 1]$, of two Gromov matrices M_1 and M_2 , with M_2 being a diagonal matrix. Let the trees corresponding to M_α , M_1 and M_2 be T_α, T_1 , and T_2 , respectively. For any $U = \{u_1, u_2, u_3\}$, its type in T_α is the same as its type in T_1 . This observation is not true in general if M_2 is not diagonal. Instead, we have the following weaker statement regarding the convex combination of an arbitrary finite set of Gromov matrices and type.

Proposition 3. *Let $\{M_1, \dots, M_k\}$ be a finite set of Gromov matrices with corresponding base trees $\{T_1, \dots, T_k\}$ with the common base vertex s and base set V . Consider $U = \{u_1, \dots, u_n\} \subset V$ a subset of distinct vertices. For any convex combination weight vector α , let M_α and M'_α be the convex and G-convex combination of $\{M_1, \dots, M_k\}$, respectively. Suppose T'_α is the tree corresponding to M'_α . For any triplet $\{u_i, u_j, u_l\} \subset U$, if*

$$M_\alpha(i, j) = M'_\alpha(i, j) \geq M'_\alpha(i, l) = M'_\alpha(j, l), \quad (2)$$

then a type of $\{u_i, u_j, u_l\}$ in T'_α is the same as its type in one of $T_1, \dots, T_k$.

Proof: From (2), we can take $\{u_i, u_j\} \cup \{u_l\}$ as a type in T'_α . As $M_\alpha(i, j) \geq M'_\alpha(i, l) = M'_\alpha(j, l)$ and each entry of M'_α is at least as large as the corresponding entry of M_α , we have $M_\alpha(i, j) \geq M_\alpha(i, l)$ and $M_\alpha(i, j) \geq M_\alpha(l, j)$.

Suppose that no type of $\{u_i, u_j, u_l\}$ in T'_α is the same as its type in any of $\{T_1, \dots, T_k\}$, i.e., for each $T_h \in \{T_1, \dots, T_k\}$, $\{u_i, u_j\} \cup \{u_l\}$ is not a type in T_h . Therefore in T_h , we have either $(u_i, u_l)_s > (u_i, u_j)_s$ or $(u_j, u_l)_s > (u_i, u_j)_s$ from the three-point condition. Taking convex combination, we have either $M_\alpha(i, l) > M_\alpha(i, j)$ or $M_\alpha(l, j) > M_\alpha(i, j)$. This gives a contradiction. ■

Proposition 3 places restrictions on T'_α , the tree corresponding to a G-convex combination M'_α . In particular, certain triplet node types must come from one of the components forming the G-convex combination, which corresponds to a spanning tree in the graph. Heuristically, taking

G-convex combinations has two basic effects: (1) re-scaling distance and (2) mixing up types of the spanning trees in the components forming the G-convex combination. We illustrate the concepts and ideas of this section by the following example.

Example 2. Consider Fig. 6. Let T_1 be the tree with Gromov matrix

$$M_1 = \begin{bmatrix} 4 & 1 & 3 & 1 \\ 1 & 4 & 1 & 1 \\ 3 & 1 & 4 & 1 \\ 1 & 1 & 1 & 4 \end{bmatrix},$$

and T_2 be the tree with Gromov matrix

$$M_2 = \begin{bmatrix} 4 & 1 & 1 & 1 \\ 1 & 4 & 3 & 2 \\ 1 & 3 & 4 & 2 \\ 1 & 2 & 2 & 4 \end{bmatrix},$$

both of which has base set $\{u_1, \dots, u_4\}$. In T_1 , $\{u_1, u_3, u_4\}$ is of type $\{u_1, u_3\} \cup \{u_4\}$, while in T_2 , $\{u_1, u_3, u_4\}$ is of type $\{u_3, u_4\} \cup \{u_1\}$. Hence $\{u_1, u_3, u_4\}$ are of different types in T_1 and T_2 . Let $\alpha = (1/2, 1/2)$, with the convex combination of M_1 and M_2 given by

$$M_\alpha = \begin{bmatrix} 4 & 1 & 2 & 1 \\ 1 & 4 & 2 & 1.5 \\ 2 & 2 & 4 & 1.5 \\ 1 & 1.5 & 1.5 & 4 \end{bmatrix},$$

which is not a Gromov matrix. On the other hand, the G-convex combination matrix is

$$M'_\alpha = \begin{bmatrix} 4 & 2 & 2 & 1.5 \\ 2 & 4 & 2 & 1.5 \\ 2 & 2 & 4 & 1.5 \\ 1.5 & 1.5 & 1.5 & 4 \end{bmatrix}.$$

The tree T'_α is shown in Fig. 6. In T_α , $\{u_1, u_3, u_4\}$ is of type $\{u_1, u_3\} \cup \{u_4\}$, the same as its type in T_1 .

Given two fixed Gromov matrices M_1, M_2 of the same size n , for θ varying from 0 to 1, the

Fig. 6. Illustration of T_1, T_2 and T_α in Example 2.

convex combinations M_α , where $\alpha = (\theta, 1 - \theta)$, give a linear path from M_1 to M_2 in the convex cone of positive definite symmetric matrices of size n . However, this linear path may not stay in the space of Gromov matrices. On the other hand, the family of G-convex combination matrices M'_α traces a continuous path between the end points M_1 and M_2 , as shown in the following theorem.

Theorem 2. *The family $\{M'_\alpha : \alpha = (\theta, 1 - \theta), \theta \in [0, 1]\}$ of G-convex combinations of the Gromov matrices M_1 and M_2 traces a piecewise linear path from M_1 to M_2 . In particular, it is continuous in θ in the space of Gromov matrices.*

Proof: See Appendix C. ■

In the following, we illustrate Theorem 2 using a toy example.

Example 3. *Consider two Gromov matrices*

$$M_1 = \begin{bmatrix} d_1 & x_1 & x_2 \\ x_1 & d_2 & x_2 \\ x_2 & x_2 & d_3 \end{bmatrix} \text{ and } M_2 = \begin{bmatrix} d'_1 & x'_1 & x'_1 \\ x'_1 & d'_2 & x'_2 \\ x'_1 & x'_2 & d'_3 \end{bmatrix}$$

such that $x_1 > x_2$ and $x'_1 < x'_2$. According to Definition 3, this is a case when their base sets are of different types (the other case is when the inequalities are reversed and the discussions are similar). For $\theta \in [0, 1]$ and $\alpha = (\theta, 1 - \theta)$, the convex combination of M_1 and M_2 is given

by

$$M_\alpha = \begin{bmatrix} \theta d_1 + (1-\theta)d'_1 & \theta x_1 + (1-\theta)x'_1 & \theta x_2 + (1-\theta)x'_1 \\ \theta x_1 + (1-\theta)x'_1 & \theta d_2 + (1-\theta)d'_2 & \theta x_2 + (1-\theta)x'_2 \\ \theta x_2 + (1-\theta)x'_1 & \theta x_2 + (1-\theta)x'_2 & \theta d_3 + (1-\theta)d'_3 \end{bmatrix}.$$

It is clear that $M_\alpha(1,3) < \min\{M_\alpha(1,2), M_\alpha(2,3)\}$. The matrix M_α is not a Gromov matrix. To construct the G -convex combination M'_α , we replace $M_\alpha(1,3)$ by $\min\{M_\alpha(1,2), M_\alpha(2,3)\}$. It can be shown that $M_\alpha(1,2) = M_\alpha(2,3)$ if and only if

$$\theta = \theta_* := \frac{x'_2 - x'_1}{(x_1 - x_2) + (x'_2 - x'_1)} \in (0, 1).$$

Therefore, for $\theta \in [0, \theta_*]$, we have

$$M'_\alpha = \begin{bmatrix} \theta d_1 + (1-\theta)d'_1 & \theta x_1 + (1-\theta)x'_1 & \theta x_2 + (1-\theta)x'_2 \\ \theta x_1 + (1-\theta)x'_1 & \theta d_2 + (1-\theta)d'_2 & \theta x_2 + (1-\theta)x'_2 \\ \theta x_2 + (1-\theta)x'_2 & \theta x_2 + (1-\theta)x'_2 & \theta d_3 + (1-\theta)d'_3 \end{bmatrix}$$

and for $\theta \in [\theta_*, 1]$,

$$M'_\alpha = \begin{bmatrix} \theta d_1 + (1-\theta)d'_1 & \theta x_1 + (1-\theta)x'_1 & \theta x_1 + (1-\theta)x'_1 \\ \theta x_1 + (1-\theta)x'_1 & \theta d_2 + (1-\theta)d'_2 & \theta x_2 + (1-\theta)x'_2 \\ \theta x_1 + (1-\theta)x'_1 & \theta x_2 + (1-\theta)x'_2 & \theta d_3 + (1-\theta)d'_3 \end{bmatrix}.$$

We see that as θ increases from 0 to 1, M'_α moves along a linear path first from M_1 to M'_{θ_*} , and then from M'_{θ_*} to M_2 . From the expressions of M_α and M'_α , we see that they agree with each other only when $\theta = 0, 1$. Therefore, the convex combinations of M_1 and M_2 for any $\theta \in (0, 1)$ are not Gromov. For a graphical illustration, see Fig. 7(a).

Since the path $\{M'_\alpha : \alpha = (\theta, 1-\theta), \theta \in [0, 1]\}$ is piecewise linear in θ , we can define the *turning points* as those M'_α such that in a small neighborhood of which, the path fails to be linear. Inspired by the above example, we make the following observation.

Corollary 3. Consider the family $\{M'_\alpha : \alpha = (\theta, 1-\theta), \theta \in [0, 1]\}$ of G -convex combinations of the Gromov matrices M_1 and M_2 and suppose N_1 and N_2 are two successive turning points with corresponding base trees T_1 and T_2 . Then any triplet $U = \{u_1, u_2, u_3\}$ of distinct vertices in the base set has the same type in T_1 and T_2 .

Fig. 7. The convex combination M_α gives a linear path between the matrices M_1 and M_2 in the vector space of $n \times n$ matrices. We illustrate the simple case where both M_1 and M_2 are 3×3 matrices in Example 3. We also indicate the shape of the corresponding base trees at the turning point and the end points of the piecewise linear path.

Proof: Suppose there exists a triplet $U = \{u_1, u_2, u_3\}$ that has different types in T_1 and T_2 . Then as discussed in Example 3, convex combinations of T_1 and T_2 are not Gromov matrices. Therefore, there must be other turning points between N_1 and N_2 , and it contradicts our assumption that N_1 and N_2 are successive turning points. ■

The corollary suggests the following intuition: at each turning point, there is a transition of some types of triples, and it is the place where several branches merge together exactly.

To end this subsection, we make a comparison between the convex combination M_α and G-convex combination M'_α , and discuss the advantages of each approach.

First, suppose we consider two general Gromov matrices M_1, M_2 and a diagonal one D . We form both the convex combination M_α and G-convex combination M'_α . According to Theorem 2, if we place them in the space of square matrices, they look like the bounded regions in Fig. 8. The shapes differ slightly, but are still quite similar. If we want to use either M_α or M'_α to approximate another *matrix* of the same size, the result of the two approaches should be comparable.

Both convex and G-convex combinations have the following advantages in network inference and estimations:

- (a) Interpolation with uniform selections of α allows us to select candidates uniformly in the space of symmetric matrices.
- (b) Even if the network topology is missing, estimations can still be performed if a few selected

Fig. 8. The convex combination ((a)) and G-convex combination ((b)) of two Gromov matrices M_1, M_2 and a diagonal Gromov matrix D , placed in the vector space of square matrices. In (a), the shape is a genuine planar triangle, while in (b), the shape is not necessary planar. It is because the turning points of the path connecting M_1 and M_2 may not stay in a common plane.

spanning trees are given.

Additional details shall be provided in Section V in conjunction with applications.

Yet, due to differences in the constructions, each approach has its own advantages. We have the following considerations:

- (a) The computational cost of forming M_α is lower than that for computing M'_α .
- (b) If the cost function varies smoothly w.r.t. the matrix entries, continuous optimization techniques (e.g., convex optimization) can be used to optimize over M_α . This is more difficult for M'_α as it does not have an analytical form.
- (c) Spectral properties of M_α are better understood, by tools such as the Weyl inequality.
- (d) The main disadvantage of the convex combination M_α is that part of the geometric information is lost; and we are not able to recover any tree in general. On the other hand, for each α , the G-convex combination M'_α gives a genuine Gromov matrix of a weighted tree. Therefore, the geometric content is completely preserved and we are able to reconstruct the associated tree with ease (see Appendix D for a discussion). We point out here that M'_α itself may not be a subtree of G . However, M'_α serves as a good approximation of a spanning tree.

B. A Case Study on Information Propagation Paths

As the approach presented in the paper is motivated by information propagation on networks, we analyze and discuss a case study based on information propagation paths. For a graph G and

a source node $v \in G$, we generate propagation times on each edge in G independently using a truncated Gaussian distribution. Let T be a shortest path tree from v , which can be interpreted as the *information propagation path* from v . Let M be the associated Gromov matrix.

We find a random BFS tree T_0 based at v . Let M_0 be its Gromov matrix and $d_0 = \|M - M_0\|_2$ be the L^2 norm of the difference between M and M_0 . We choose another BFS tree T_1 based at v with the associated matrix M_1 and let D be the diagonal matrix of M_1 . Now we form G-convex combinations between M_0 and M_1 with parameter α to obtain M_α ; and then form G-convex combinations between M_α with D with parameter β to obtain $M_{\alpha,\beta}$. Let $d = \min_{\alpha,\beta} \|M - M_{\alpha,\beta}\|_2$. We have $d_0 \geq d$ and we want to know how large is the ratio $(d_0 - d)/d$. A larger ratio means the Gromov method gives a better approximation of T .

Fig. 9. Plot of the ratio $(d_0 - d)/d$ against propagation mean μ .

We perform simulations on both synthetic Erdős-Rényi (ER) graphs and the Enron email network² (as an example of a scale-free graph) with 500 nodes. For convenience, we fix the variance σ^2 of the truncated Gaussian distribution as 1 and vary the mean μ . Intuitively, if the mean is larger, the information propagation path T looks more like a BFS tree. The simulation results are plotted in Fig. 9. We observe that if μ is larger (i.e., the actual information propagation path T resembles a BFS tree more closely), then our approach gives a much better approximation of T than simply choosing a random BFS tree T_0 . The intuition is as follows: even though the randomly chosen BFS trees T_0, T_1 are not close to T , there exists a projection of M in the convex region formed by M_0, M_1 , and D (see Fig. 10). This example suggests that by using

²<https://snap.stanford.edu/data/email-Enron.html>

Fig. 10. Illustration of the explanation of the observation regarding Fig. 9.

G-convex combinations to approximate the information propagation path T in problems where T is unknown *a priori* is a better approach than the spanning tree heuristic.

V. APPLICATIONS OF THE GROMOV METHOD

The theory developed in this paper can be used as an alternative to a spanning tree heuristic in network inference and estimation problems. In the spanning tree heuristic, given an estimator ϕ that outputs a cost given an input tree that satisfies certain criteria according to the problem of interest, for a general graph G , we randomly select a spanning tree with the same criteria and use that as an input to ϕ . Multiple such spanning trees maybe sampled to optimize ϕ . For our *Gromov method*, instead of randomly selecting a spanning tree, we choose two spanning trees T_1 and T_2 with associated Gromov matrices M_1 and M_2 . Let D be the diagonal matrix taking the diagonal of M_1 and form $\mathbf{M} = \{M_1, M_2, D\}$. We then apply ϕ to either the convex combination M_α or G-convex combination M'_α formed from $\mathbf{M}$. The advantages of the Gromov method are as follows:

- (a) Taking the convex or G-convex combination gives us a larger family of approximate spanning trees, while retaining certain structural features of the ambient graph G (see Corollary 1, Fig. 3 and Proposition 3). Standard optimization techniques may then be applied to optimize ϕ over this family.
- (b) In some applications, we may not have access to all the spanning trees satisfying the problem criteria, or it may be computationally complex to find such spanning trees (cf. the timestamp variant of the problem in Section V-B). It becomes difficult to construct many spanning

trees using the tree heuristic. With the Gromov method, we mitigate this problem by using only a small set of spanning trees and then forming convex or G-convex combinations from them.

In the following, we present several network inference applications to illustrate the use of the Gromov method.

A. Information Acquisition Order

Suppose that information is propagated stochastically from a source node s in a graph G , where the propagation time distribution along each edge is known. An important application is knowing if on average a node u lies on the propagation path from s to another node v . For example, in viral marketing and social learning (e.g., [2], [5], [7], [24]), we are interested to find those nodes in a social network that act as the gatekeepers of information propagation. In infection control and monitoring (e.g., [15], [25]–[28]), we are interested to identify those nodes in a network with the highest probability of acquiring the infection and spreading it to others in the network so that we can add monitoring and countermeasures at these nodes.

Information propagation from s follows a random spanning tree T . Computing the probability that $u \in [s, v]$, where $[s, v]$ is the unique path in T connecting s and v is intractable for a dense graph G . Therefore, we sample enough random spanning trees containing s, u and v . For each such tree T , we decide if u is on the unique path $[s, v]$ connecting s and v or not. We use the *empirical probability* of instances of $u \in [s, v]$ as the ground truth.

On the other hand, we may sample a very small amount of spanning trees, and use G-convex combinations to synthesize more. Again, we are able to estimate the empirical probability of instances of $u \in [s, v]$. It is compared with the ground truth to examine the accuracy. It is interesting to notice that to perform this estimation, we do not even need to know the network topology, provided we are given a few samples. In this problem, we need to use G-convex combinations, as geometric information of the synthesized trees is used.

We performed simulations on three types of dense graphs: the Enron email network, a sample Facebook network³ and the complete graph, as an extreme case. For each simulation, we sample three spanning trees and form 10 G-convex combinations between each pair of sampled spanning

³<https://snap.stanford.edu/data/egonets-Facebook.html>

trees, giving approximately 30 synthesized trees. The ground truth is obtained by averaging over 200 – 500 samples depending on the density of the network.

It is useful to notice that the size of the network is not a crucial factor here since we only need to make sure the spanning tree is large enough to contain the three involved nodes. On the other hand, the ratio r between the average node degree and the number of nodes gives an important indication of the density of the graph.

The simulation results are shown in Table I. We see that the Gromov method performs reasonably well and yields a good estimation with a limited number of samples.

	Degree-node ratio r	Accuracy
Email network	0.094	95.26%
Facebook network	0.268	91.11%
Complete graph	≈ 1	94.02%

TABLE I
ACCURACY OF THE GROMOV METHOD IN ESTIMATING INFORMATION ACQUISITION ORDER.

B. Network Source Identification

Next, we consider the problem posed in Example 1 in the introduction. We start with the case where a snapshot of the infection status of each node is observed. We assume that infection propagation along each edge follows an exponential distribution with mean 1. Suppose we are given a snapshot $I \subset V$ of all the infected nodes. We want to estimate the identity of the source node. One possible approach is estimator based. An estimator $e(s, T_s)$ is a real valued function on each candidate source node s and a spanning tree T_s of I rooted at s . The source is found by minimizing $e(\cdot, \cdot)$ over all s . In the spanning tree heuristic adopted by [9], for a general graph, a random BFS tree T_s is usually chosen as the second argument of $e(\cdot, \cdot)$, which might be a source of error in the estimation.

Various estimators have been studied in the literature [9], [17], [29], [30], and for demonstration purposes, we choose the centroid $e_C(\cdot, \cdot)$ as an example. The centroid $e_C(s, T)$ (see [17]) is defined as the maximal size, i.e., the sum of all the edge weights, of connected components of $T \setminus \{s\}$. The Gromov method can be applied directly. We run simulations on both synthetic and real networks: Barabási-Albert (BA) graphs with 500 vertices and average degree 4, ER graphs with 500 vertices and average degree 4, and the Enron email network with 670 vertices and average degree 9.86.

In each simulation, we infect 20% to 30% of the vertices; and we evaluate the performance by computing the average distance between the true source and the estimated source. The error reduction rates when using the Gromov method compared to the tree heuristic are shown in Table II. We see noticeable improvement of the Gromov method in all the cases.

	Average degree	Size	Error reduction
BA graph	4	500	12.4%
ER graph	4	500	18.6%
Email network	9.86	670	12.7%

TABLE II

ERROR REDUCTION OF THE GROMOV METHOD OVER THE SPANNING TREE HEURISTIC IN NETWORK SOURCE ESTIMATION.

Another variant of the problem is source estimation with observed infection timestamps. Here, we assume that a small percentage of the infected nodes are observed, together with their respective infection timestamps. A maximal-likelihood based estimator (MLE) can be derived. Therefore, we are able to apply the Gromov based method (using convex combination), as in the snapshot observation based estimation described above. We compare the Gromov method with the BFS tree based approach (called BFS-MLE), as well as other approaches: GAU [10] and TRBS [31], on various networks. The results are shown in Fig. 11, which is reproduced from [20] here for completeness. We vary the number of nodes with observed timestamps. We observe significant performance improvement using the Gromov method in most cases.

C. Data Center Placement

In this application, we consider the problem of determining the optimal placement of data centers in a large network. Mathematically, the problem can be described as follows. The network is described by a weighted graph $G = (V, E)$. For each node $v \in V$, a non-negative number $w(v)$ is associated to it to indicate the service demand at v . Given a subset $S \subset V$ and $v \in V$, let $s(v, S) = \arg \min_{s \in S} d_G(s, v)$, i.e., the node in S closest to v . The overall weighted cost of serving V by S is defined as $\text{cost}(S) = \sum_{v \in V} w(v) d_G(s(v, S), v)$. We want to find a subset $\hat{S} = \arg \min_{S \subset V, |S|=k} \text{cost}(S)$, where k is the number of data centers.

There are both centralized and localized approaches to solve the problem. One localized approach is proposed in [32]. To highlight the essential changes required to accommodate the Gromov method, we briefly recall that [32] proposes to partition G into k connected subgraphs, and place a data center in each subgraph. To do so, a single spanning tree is found. Therefore, the

Fig. 11. Performance comparison for the network source estimation problem with timestamps.

Gromov method can be applied to replace this step by using a convex combination of different spanning trees. We call it the Gromov-localized method.

To study the performance of this approach, we compare it with the centralized greedy algorithm proposed in [33]. We run simulations on both grid networks and CAIDA AS graphs (see [34]). We vary both the graph size (100 to 400 nodes) and number of data centers (1%, 2% of the total number of nodes) for each graph type. The service demand for each node is generated according to the Pareto distribution, which is a power-law distribution used to model the situation where a small number of nodes generate most of the service demand.

For each instance, we compute the estimated cost c_1 for the centralized greedy method, and c_2 for the Gromov-localized method. The performance of the two methods are compared by taking the average of the ratio $r_c = c_1/c_2$. The simulation results are shown in Fig. 12. We see that the Gromov-localized method has a better performance in almost all the cases (average cost ratio $r_c - 1 > 0$).

Fig. 12. Performance comparison between the Gromov-localized method and the centralized greedy method on grid networks and AS graphs.

VI. CONCLUSION

In this paper, using the Gromov matrix interpretation of trees, we have proposed a modified version of the commonly used spanning tree heuristic, which we call the Gromov method, in network inference problems. We presented both necessary and sufficient conditions for a matrix to be a Gromov matrix of a weighted tree, followed by a demonstration on how to form convex combinations of Gromov matrices. The Gromov method proposed is based on optimizing the network inference objective function over a parametrized family of Gromov matrices. We give some applications of the Gromov method on network inference and estimation. As the proposed Gromov method provides a general framework, it is of interest to explore other network inference and estimation applications in future works. Moreover, how to choose the appropriate matrices or spanning trees in forming the convex combinations is also an interesting and important topic to explore.

APPENDIX A

PROOF OF PROPOSITION 1

Suppose that the base of M is (T, s, V) . We first note that conjugation by permutation matrices is equivalent to a re-ordering of the indices of M . Therefore, we can ignore the ordering of the indices in our proof. To prove the proposition, it suffices to prove that the weighted tree with base (T, s, V) can be obtained from the Gromovication operations starting from $(\{s\}, s, \emptyset)$.

Fig. 13. Illustration of the geometric constructions corresponding to the Gromov operations.

We first observe that each Gromov operation on Gromov matrices corresponds to the construction of a new base from the bases associated with the input Gromov matrices as follows (see Fig. 13 for an illustration).

- Initialization: Given the base $(\{s\}, s, \emptyset)$ and $a > 0$, we form a tree by attaching an edge e of weight a to s . Denote the other end of e by v and let $T = (\{s, v\}, e)$. Then the base of the initialization is $(T, s, \{v\})$.
- Direct sum: Given the bases (T_L, s_L, V_L) and (T_N, s_N, V_N) corresponding to the Gromov matrices L and N respectively, we form a new tree T' by joining the two trees T_L and T_N at their base vertices and identifying both s_L and s_N as a single base vertex s' . A base of $L \oplus N$ is then $(T', s', V_L \cup V_N)$.
- Extension I (with parameter $a > 0$): Given a base (T_N, s_N, V_N) corresponding to the Gromov matrix N , we form a new tree T' by attaching a path P of length a at s_N , and letting s' be the other endpoint of P . Then (T', s', V_N) is a base of $\phi_a(N)$.
- Extension II (with parameters $a \geq b > 0$): Given a base (T_N, s_N, V_N) corresponding to the Gromov matrix N , we form a new tree T' by attaching a path P of length a at s_N as in extension I, with s' being the other endpoint of P . The path P is constructed to have a vertex v whose distance to s' is b (it is possible that $v = s_N$). Then, the base $(T', s', V_N \cup \{v\})$ corresponds to $\phi_{a,b}(N)$.

We now proceed to prove Proposition 1 for the base (T, s, V) by induction on $n = |V|$. As we assume that T is non-empty, V is non-empty. The case $|V| = 1$ requires an initialization step. Suppose that the proposition is true when the base set has less than n vertices. Let $v \in V$ be a

node such that $[v, s] \cap V = \{v\}$. There are two cases to consider (see Fig. 14 for an illustration):

- (a) The path $P = (v, s]$ does not contain any vertex of degree greater than 2. Let $T' = T \setminus P$, $s_{T'} = v$ and $V_{T'} = V_T \setminus \{v\}$. As $|V_{T'}| = |V_T| - 1$, by the induction hypothesis, we can obtain $(T', s_{T'}, V_{T'})$ by the Gromovication operations. Moreover, (T, s, V) can be constructed from $(T', s_{T'}, V_{T'})$ by an extension II.
- (b) The path $P = (v, s)$ contains of a vertex u of degree greater than 2. By our choice of v , the node $u \notin V$. We can always find two connected subtrees T_1 and T_2 of $T \setminus P$ such that:
 - (i) $T_1 \cap T_2 = u$;
 - (ii) $T_1 \cup T_2 = T \setminus P$;
 - (iii) $T_i \cap V \neq \emptyset$, for $i = 1, 2$.

Let $s_{T_1} = s_{T_2} = u$; and $V_{T_i} = T_i \cap V$, for $i = 1, 2$. The induction hypothesis implies that both $(T_i, s_{T_i}, V_{T_i}), i = 1, 2$ can be obtained from Gromovication operations. Moreover, (T, s, V) can be obtained from $(T_i, s_{T_i}, V_{T_i}), i = 1, 2$ by a direct sum followed by possibly an extension I.

The proof is now complete.

Fig. 14. Illustration of the two cases in the induction step.

APPENDIX B

PROOF OF PROPOSITION 2

- (a) This is obvious.
- (b) Recall that a special case of Weyl's inequality (cf. [35]) asserts the following: For two symmetric matrices M and N of the same size, the inequality

$$\lambda_{\min}(M + N) \geq \lambda_{\min}(M) + \lambda_{\min}(N) \quad (3)$$

holds. In view of Weyl's inequality, it suffices to note that the $n \times n$ matrix with identical entries a has two eigenvalues na and 0 .

- (c) Let $\mathbf{1}_n$ be the $n \times n$ square matrix with all entries 1. If $a > b$, we form two $(n+1) \times (n+1)$ matrices: $M_1 = M \oplus (b - b^2/a)$; and M_2 has the $n \times n$ block $a\mathbf{1}_n$ as its top-left submatrix, b^2/a in the bottom-right corner, and the remaining entries b . The column rank of M_2 is 1 and it is easy to check that $\lambda_{\min}(M_2) = 0$. Moreover, from item (a), $\lambda_{\min}(M_1) = \min\{\lambda_{\min}(M), b - b^2/a\}$. Therefore, as $\phi_{a,b}(M) = M_1 + M_2$, we have the desired inequality

$$\lambda_{\min}(\phi_{a,b}(M)) \geq \min\{\lambda_{\min}(M), b - b^2/a\}$$

by Weyl's inequality (3).

Suppose $a = b$. Let $\alpha = \lambda_{\min}(M)/a$. We form two $(n+1) \times (n+1)$ matrices: $M_1 = M \oplus (a\alpha)$; and M_2 , which has $a(1 - \alpha)$ in the bottom-right corner and a everywhere else. As $\phi_{a,a}(M) = M_1 + M_2$, by Lemma B.1 below and Weyl's inequality, we have

$$\begin{aligned} \lambda_{\min}(\phi_{a,a}(M)) &\geq \lambda_{\min}(M_1) + \lambda_{\min}(M_2) \\ &= a\alpha + a \frac{n+1-\alpha - \sqrt{(n+1-\alpha)^2 + 4n\alpha}}{2} \\ &= a \cdot \frac{n+1+\alpha - \sqrt{(n+1+\alpha)^2 - 4\alpha}}{2} \\ &\geq \frac{a\alpha}{n+1+\alpha} = \frac{\lambda_{\min}(M)}{n+1+\lambda_{\min}(M)/a}. \end{aligned}$$

The proof of the proposition is now complete.

Lemma B.1. *Suppose that M is the $n \times n$ matrix whose bottom-right corner is $1 - \alpha$ for some $\alpha > 0$, and has 1 everywhere else. Then*

$$\lambda_{\min}(M) = \frac{n - \alpha - \sqrt{(n - \alpha)^2 + 4(n - 1)\alpha}}{2}.$$

Proof: It is enough to show that the characteristic polynomial of M is $(-1)^n \lambda^{n-2} (\lambda^2 - (n - \alpha)\lambda - (n - 1)\alpha)$. We give a sketch of the proof with some calculation details omitted. First we note that M has $n - 1$ identical columns, the characteristic polynomial takes the form $(-1)^n \lambda^{n-2} (\lambda^2 - a\lambda - b)$, where the coefficient a is the trace $n - \alpha$.

Let $M' = M - \lambda I_n$, where I_n is the $n \times n$ identity matrix. To determine b , let $C(i, j)$ be the (i, j) -th cofactor of M' ; and $M'(i, j)$ the (i, j) -th entry of M' . The determinant $\det(M') =$

$\sum_{1 \leq j \leq n} M'(1, j)C(1, j)$. The summand $M'(1, 1)C(1, 1) = (1 - \lambda)C(1, 1)$ can be computed by induction as

$$(1 - \lambda)(-1)^{n-1}\lambda^{n-3}(\lambda^2 - (n - 1 - \alpha)\lambda - (n - 2)\alpha).$$

For the remaining summands, only the leading coefficient of λ^{n-2} contributes to b , which is either 1 or -1 ; and the coefficient of λ^{n-2} of $\sum_{1 < j \leq n} M'(1, j)C(1, j)$ is $(-1)^{n-1}(n - 1)$. It is now easy to obtain that $b = (n - 1)\alpha$. $\blacksquare$

APPENDIX C

PROOF OF THEOREM 2

We first prove an elementary lemma.

Lemma C.1. *For a triplet of real numbers $A = \{a_1, a_2, a_3\}$, the new triplet $A' = \{a'_1, a'_2, a'_3\}$ defined by $a'_i = \max\{a_i, \min(A \setminus \{a_i\})\}$ satisfies the following properties:*

- (a) $|A \cap A'| \geq 2$;
- (b) $\max(A) = \max(A')$;
- (c) *The triplet A' satisfies the three-point condition.*

Proof: Without loss of generality, we assume that $a_1 \geq a_2 \geq a_3$. It is easy to verify that $a'_1 = a_1, a'_2 = a_2$ and $a'_3 = a_2$. Therefore, the lemma follows. $\blacksquare$

For convenience, we call a'_i the *max-min* of a_i w.r.t. A . Suppose we have a pair of functions $a(\alpha)$ and $b(\alpha)$. If both of them are piecewise linear continuous in α , then so are $\max(a, b)$ and $\min(a, b)$. Similarly, suppose we have functions $a_1(\alpha), a_2(\alpha), a_3(\alpha)$ such that all of them are piecewise linear continuous in α . Then the same holds for the max-min of $a_i(\alpha), i = 1, 2, 3$, w.r.t. $\{a_1(\alpha), a_2(\alpha), a_3(\alpha)\}$.

We now proceed with the proof of Theorem 2. We have the following alternative (though inefficient) way of obtaining M'_α from the convex combination M_α . The matrices constructed below depends on α , but for convenience, we suppress α in the notations. We start with $N_0 = M_\alpha$ and N_i is obtained from N_{i-1} as follows: given $j < k$ and $l \neq j, k$, we first form the triple $A_{j,k,l} = \{N_{i-1}(j, k), N_{i-1}(l, j), N_{i-1}(l, k)\}$. Next, we find $a_{j,k}^l$ as the max-min of $N_{i-1}(j, k)$ w.r.t. $A_{j,k,l}$. The (j, k) -th entry of N_i is taken as $\max_{l \neq j, k} a_{j,k}^l$. During this process, the only functions involved are max and min. Therefore, if the entries of N_{l-1} are piecewise linear in the parameter α , so are the entries of N_l . Hence N_l itself is piecewise linear in α when considered as an element of the vector space of $n \times n$ square matrices.

To conclude the proof of the theorem, we need to show two additional assertions:

- (i) The sequence of matrices $N_i, i \geq n$ stabilizes (the entries do not change in the next iteration) after a fixed number of iterations.
- (ii) The stabilized matrix is M'_α .

For (i), we make the following observation: the largest off-diagonal entries of N_0 do not change in subsequent iterations. Denote by S_i the positions of the entries of N_i that do not change in all subsequent iterations, which is non-empty by the case $i = 0$. On the other hand, the largest off-diagonal entries of N_{i+1} with positions different from S_i do not change in all subsequent iterations. Therefore $|S_{i+1}| > |S_i|$ unless $N_{i+1} = N_i$. Therefore the sequence of matrices stabilizes within $n(n-1)/2$ iterations.

For (ii), it is easy to see that the construction given in Section VI is merely an economized alternative for M'_α . The result thus follows.

APPENDIX D

SOME GEOMETRIC CONSTRUCTIONS

Suppose M is a Gromov matrix with base (T, s, V) , where $V = \{v_1, \dots, v_n\}$. For each vertex pair v_i, v_j , the distance $d_T(v_i, v_j)$ between them can be recovered as $M(i, i) + M(j, j) - 2M(i, j)$. The nodes in V uniquely determine T as $V \cup \{s\}$ span T . However, we are not able to recover the (weighted) adjacency matrix of T directly using such information, as V may not contain all the vertices of T in the usual sense (for a simple example, see Fig. 6). On the other hand, in certain applications, we are interested in the relative positions of vertices of V on T , instead of the relative distance (e.g., some applications may require only knowledge of the number of neighbors of certain vertices, or the size of the connected components after removing a particular node). In this appendix, we discuss certain geometric constructions based on (T, s, V) , or equivalently M , which allows us to explore the relative positions of the vertices of V .

We first introduce a graph G_V as follows: the size of G_V is $|V| = n$ and let $U = \{u_1, \dots, u_n\}$ be the vertex set of G_V . Two vertices u_i and u_j are connected by an edge in G_V if and only if $[v_i, v_j] \cap V = \{v_i, v_j\}$ in T . The weight of each edge of G_V is set to be 1, and the distance metric on G_V is denoted by $d_{G_V}(\cdot, \cdot)$.

For each path P (not required to be simple) in G_V , we form an associated path P' in T as follows: if P is obtained from concatenating edges (u_i, u_j) , we construct P' by concatenating simple paths $[v_i, v_j]$. If P with length l is a path connecting u_i and u_j such that $d_{G_V}(u_i, u_j) = l$,

Fig. 15. In tree T , consider $V = \{v_1, v_2, v_3\}$. The associated G_V (shown on the right) is no longer a tree.

then we call P a *geodesic* path for convenience. One should take note here that G_V is not a tree in general (cf. Fig. 15), and there can be multiple geodesic paths between two nodes.

Lemma D.1. *If P is a geodesic path connecting u_i and u_j , then the associated path P' in T is simple.*

Proof: Let the length of P be l . We prove the claim by induction on l . The case $l = 1$ clearly holds by definition.

Suppose the claim holds for $l = t$. Consider $l = t + 1$. Let $P_1 = [u_i, u_k]$ be the subpath of P starting from u_i of length t . By the induction hypothesis, the associated path P'_1 in T is simple, connecting v_i and v_k . If the intersection $[v_k, v_j] \cap P'_1 = \{v_k\}$ in T , then P' as the concatenation of P'_1 and $[v_k, v_j]$ is simple; and this proves the lemma.

Otherwise, $[v_k, v_j] \cap P'_1 \neq \{v_k\}$ (see Fig. 16 for an illustration). In this case, there exists a $v_r \neq v_k$ in P' and $v_r \in [v_k, v_j] \cap P'_1$. We can form another path P_2 consisting of $[u_i, u_r]$ concatenated with $[u_r, u_j]$ in G_V . The path P_2 is of length strictly smaller than l ; and hence $d_{G_V}(u_i, u_j) < l$. This contradicts the assumption that P is a geodesic path. ■

Since G_V may not be a tree (cf. Fig. 15), and we have the following weaker substitute.

Corollary D.1. *For each $u \in U$, there is a unique BFS tree of G_V based at u .*

Proof: Suppose on the contrary that for $u_i \in U$ there are two distinct BFS trees T_1 and T_2 of G_V . This means that there is a vertex $u_j \neq u_i \in U$ such that the following holds:

- (a) The path $[u_i, u_j]$ in T_1 and T_2 are distinct; and denote them by P_1 and P_2 respectively.
- (b) P_1 and P_2 are of the same length $d_{G_V}(u_i, u_j)$.

Let P'_1 and P'_2 be their associated paths (connecting say v_i and v_j) in T respectively. As P_1 and P_2 are distinct, so are P'_1 and P'_2 . Moreover, by Lemma D.1, both P'_1 and P'_2 are simple

Fig. 16. Illustration of the case $[v_k, v_j] \cap P'_1 \neq \{v_k\}$ in the proof of Lemma D.1.

paths. This is absurd, as T is a tree and there is a unique simple path connecting v_i and v_j . This concludes the proof of the corollary by contradiction. ■

From this result, we see that G_V resembles a tree in the sense that each node has a unique BFS tree. It is an important feature to handle information propagation. On the other hand, U contains all the nodes of G_V . Therefore, we may use G_V to study the relative positions of nodes in V of T , as well as other combinatorial properties.

Now we indicate how to obtain the adjacency matrix A of G_V from the Gromov matrix M . To determine the (i, j) -th entry $A(i, j)$ of A , consider v_i and v_j in T . As we have demonstrated, the distance $d_T(v_i, v_j)$ can be recovered from M . Moreover, recall that T is a tree. Therefore $A(i, j) = 1$ if and only if for each $1 \leq k \neq i, j \leq n$, $d_T(v_i, v_j) \neq d_T(v_i, v_k) + d_T(v_j, v_k)$; or equivalently,

$$M(k, k) + M(i, j) \neq M(i, k) + M(k, j).$$

The checking involves only addition and is efficient to do.

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