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A Note on Tree Realizations of Matrices

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Abstract

It is well known that each tree metric M has a unique realization as a tree, and that this realization minimizes the total length of the edges among all other realizations of M. We extend this result to the class of symmetric matrices M with zero diagonal, positive entries, and such that $m_{ij} + m_{kl} \leq max\{m_{ik} + m_{jl}, m_{il} + m_{jk}\}$ for all distinct i, j, k, l.

Résumé

Il est bien connu qu'une matrice de distance M a une réalisation unique en tant qu'arbre, et que cette réalisation minimise la longueur totale des arêtes par rapport à toutes les autres réalisations de M. Nous étendons ce résultat à l'ensemble des matrices symétriques de diagonale nulle, ayant des entrées positives et tel que $m_{ij} + m_{kl} \leq max\{m_{ik} + m_{jl}, m_{il} + m_{jk}\}$ pour tout i, j, k, l distincts.

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1 Introduction

An $n \times n$ matrix $M = (m_{ij})$ with zero diagonal is a *tree metric* if it satisfies the following *4-point condition*:

$$m_{ij} + m_{kl} \leq max\{m_{ik} + m_{jl}, m_{il} + m_{jk}\} \qquad \forall i, j, k, l \text{ in } \{1, \ldots, n\}$$

The 4-point condition entails the triangle inequality (for $k = l$) and symmetry (for $i = k$ and $j = l$). There is an extensive literature on tree metrics; see for example [1, 2, 5, 6, 7, 8].

It is well known that a tree metric $M = (m_{ij})$ can be represented by an unrooted tree T such that $\{1, \ldots, n\}$ is a subset of the vertex set of T, and the length of the unique chain connecting two vertices i and j in T $(1 \leq i < j \leq n)$ is equal to m_{ij}.

Let $G = (V, E, d)$ be the graph with vertex set V, edge set E, and where d is a function assigning a positive length d_{ij} to each edge (i, j) of G. The length of the shortest chain between two vertices i and j in G is denoted d^G_{ij}.

Definition 1 *Let M be a symmetric $n \times n$ matrix with zero diagonal and such that $0 \leq m_{ij} \leq m_{ik} + m_{kj}$ for all i, j, k in $\{1, \ldots, n\}$. A graph $G = (V, E, d)$ is a realization of $M = (m_{ij})$ if and only if $\{1, \ldots, n\}$ is a subset of V, and $d^G_{ij} = m_{ij}$ for all i, j in $\{1, \ldots, n\}$.*

As mentioned above, tree metrics have a realization as a tree. A realization G of a matrix M is said *optimal* if the total length of the edges in G is minimal among all realizations of M. Hakimi and Yau [5] have proved that tree metrics have a unique realization as a tree, and this realization is optimal.

We propose to extend the above definition to matrices whose entries do not necessarily satisfy the triangle inequality. Given a symmetric $n \times n$ matrix $M = (m_{ij})$ with zero diagonal and positive entries, let K_M denote the complete graph on n vertices in which each edge (i, j) has length m_{ij}.

Definition 2 *Let M be a symmetric $n \times n$ matrix with zero diagonal and positive entries. A graph $G = (V, E, d)$ is a realization of $M = (m_{ij})$ if and only if $\{1, \ldots, n\}$ is a subset of V, and $d^G_{ij} = d^{K_M}_{ij}$ for all i, j in $\{1, \ldots, n\}$.*

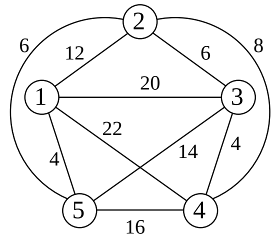
Obviously, if M satisfies the triangle inequality, then $d^{K_M}_{ij} = m_{ij}$, and Definition 2 is then equivalent to Definition 1. Figure 1 illustrates this new definition. Notice that the matrix in Figure 1 is not a tree metric, while it has a realization as a tree.

Let $\mathcal{M}_n$ denote the set of symmetric $n \times n$ matrices $M = (m_{ij})$ with zero diagonal, positive entries, and such that $m_{ij} + m_{kl} \leq max\{m_{ik} + m_{jl}, m_{il} + m_{jk}\}$ for all *distinct* points i, j, k, l in $\{1, \ldots, n\}$.

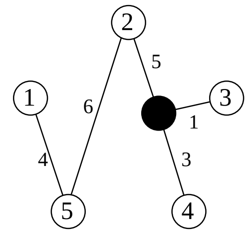
Since we only impose the 4-point condition on *distinct* points i, j, k, l, the entries of a matrix in $\mathcal{M}_n$ do not necessarily satisfy the triangle inequality. While all tree metrics

$$\begin{pmatrix} 0 & 12 & 20 & 22 & 4 \\ 12 & 0 & 6 & 8 & 6 \\ 20 & 6 & 0 & 4 & 14 \\ 22 & 8 & 4 & 0 & 16 \\ 4 & 6 & 14 & 16 & 0 \end{pmatrix}$$

A matrix M.



Its associated complete graph K_M.



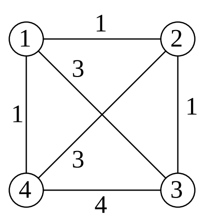
A realization of M as a tree.

Figure 1: A tree realization of a tree metric

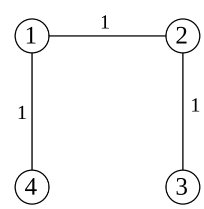
belong to $\mathcal{M}_n$, the example in Figure 2 shows that a matrix having a realization as a tree does not necessarily belong to $\mathcal{M}_n$. However, we prove in this paper that all matrices in $\mathcal{M}_n$ have a unique realization as a tree, and that this realization is optimal.

$$\begin{pmatrix} 0 & 1 & 3 & 1 \\ 1 & 0 & 1 & 3 \\ 3 & 1 & 0 & 4 \\ 1 & 3 & 4 & 0 \end{pmatrix}$$

A 4×4 matrix M that does not belong to $\mathcal{M}_4$.



Its associated complete graph K_M.



A realization of M as a tree.

Figure 2: A tree realization of a matrix that does not belong to $\mathcal{M}_n$

2 The main result

Let $M = (m_{ij})$ be any matrix in $\mathcal{M}_n$, and consider the matrix $M' = (m'_{ij})$ obtained from M by setting m'_{ij} equal to the length $d_{ij}^{K_M}$ of the shortest chain between i and j in K_M. Notice that the elements in M' satisfy the triangle inequality. In order to prove that M has a realization as a tree, it is sufficient to prove that M' is a tree metric. The proof is based on Floyd's algorithm [4] for the computation of M'.

Floyd's algorithm [4]

Set M^0 equal to M;

For $r := 1$ to n do

For all i and j in $\{1, \ldots, n\}$ do

Set m_{ij}^r equal to $min\{m_{ij}^{r-1}, m_{ir}^{r-1} + m_{rj}^{r-1}\}$;

Set M' equal to M^n;

We shall prove that each matrix M^r $(1 \leq r \leq n)$ is in $\mathcal{M}_n$. Since the entries of $M' = M^n$ satisfy the triangle inequality, we will be able to conclude that M' is a tree metric.

Theorem 1 *Let $M = (m_{ij})$ be a matrix in $\mathcal{M}_n$, and let $M' = (m'_{ij})$ be the $n \times n$ matrix obtained from M by setting $m'_{ij} = d_{ij}^{K_M}$ for all i and j in $\{1, \ldots, n\}$. Then M' is a tree metric.*

Proof. Following Floyd's algorithm, define $M^0 = M$ and let M^r be the matrix obtained from M^{r-1} by setting $m_{ij}^r = min\{m_{ij}^{r-1}, m_{ir}^{r-1} + m_{rj}^{r-1}\}$ for all i and j in $\{1, \ldots, n\}$. Given four distinct points i, j, k, l in $\{1, \ldots, n\}$, we denote $s_{ijkl}^r = m_{ij}^r + m_{kl}^r$. We prove by induction that each M^r $(r = 1, \ldots, n)$ is in $\mathcal{M}_n$. By hypothesis, $M^0 = M$ is in $\mathcal{M}_n$, so assume $M^{r-1} \in \mathcal{M}_n$. It is sufficient to show that $s_{ijkl}^r \leq max\{s_{ikjl}^r, s_{iljk}^r\}$ for all distinct i, j, k, l in $\{1, \ldots, n\}$, or equivalently, that two of the three sums s_{ijkl}^r, s_{ikjl}^r and s_{iljk}^r are equal and not less than the third.

Notice that $m_{ri}^r = m_{ri}^{r-1}$ and $m_{ij}^r \leq m_{ij}^{r-1}$ for all $1 \leq i \leq j \leq n$. Consider any four distinct points i, j, k and l. Since r is possibly one of these four points, we divide the proof into two cases.

Case A: $r \in \{i, j, k, l\}$, say $r = l$.

Since $M^{r-1} \in \mathcal{M}_n$, we may assume, without loss of generality that $s_{rijk}^{r-1} \leq s_{rjik}^{r-1} = s_{rkij}^{r-1}$. If $m_{ik}^r = m_{ik}^{r-1}$ and $m_{ij}^r = m_{ij}^{r-1}$, then $s_{rijk}^r \leq s_{rjik}^r = s_{rkij}^r$. We may therefore assume $m_{ik}^r < m_{ik}^{r-1}$. It then follows that $m_{ri}^{r-1} + s_{rjik}^{r-1} = m_{ri}^{r-1} + s_{rkij}^{r-1} < m_{ik}^{r-1} + m_{ij}^{r-1}$, which means that $m_{ij}^r = m_{ri}^{r-1} + m_{rj}^{r-1} < m_{ij}^{r-1}$. We therefore have $s_{rijk}^r \leq m_{ri}^{r-1} + m_{rj}^{r-1} + m_{rk}^{r-1} = s_{rjik}^r = s_{rkij}^r$.

Case B: $r \notin \{i, j, k, l\}$.

If $s_{ijkl}^r = s_{ijkl}^{r-1}, s_{ikjl}^r = s_{ikjl}^{r-1}$ and $s_{iljk}^r = s_{iljk}^{r-1}$, there is nothing to prove. So assume without loss of generality that $m_{ij}^r < m_{ij}^{r-1}$. Notice that if $m_{ik}^r = m_{ik}^{r-1}$, $m_{il}^r = m_{il}^{r-1}$, $m_{jk}^r = m_{jk}^{r-1}$ and $m_{jl}^r = m_{jl}^{r-1}$, then we are done. Indeed, since $M^{r-1} \in \mathcal{M}_n$ and $s_{rkij}^r < s_{rkij}^{r-1}$, while $s_{rjik}^r = s_{rjik}^{r-1}$ and $s_{rijk}^r = s_{rijk}^{r-1}$, we know from *Case A* that $s_{rjik}^{r-1} = s_{rijk}^{r-1}$. In a similar way, we also have $s_{rjil}^{r-1} = s_{rijl}^{r-1}$. Hence, $s_{rjik}^{r-1} + s_{rijl}^{r-1} = s_{rijk}^{r-1} + s_{rjil}^{r-1}$, which means that $s_{ikjl}^{r-1} = s_{iljk}^{r-1}$. Since $M^{r-1} \in \mathcal{M}_n, s_{ikjl}^r = s_{ikjl}^{r-1}, s_{iljk}^r = s_{iljk}^{r-1}$ and $s_{ijkl}^r < s_{ijkl}^{r-1}$ we conclude that $s_{ijkl}^r < s_{ikjl}^r = s_{iljk}^r$.

Without loss of generality, we can therefore assume $m_{ik}^r < m_{ik}^{r-1}$. The rest of the proof is divided into four subcases.

Case B1: $m_{jk}^{r-1} < m_{rj}^{r-1} + m_{rk}^{r-1}$ and $m_{jl}^{r-1} > m_{rj}^{r-1} + m_{rl}^{r-1}$.

Since $s^r_{rkjl} = m^{r-1}_{rk} + m^{r-1}_{rj} + m^{r-1}_{rl} > s^r_{rljk}$, we know from *Case A* that $s^r_{rjkl} = s^r_{rkjl}$, which means that $m^r_{kl} = m^{r-1}_{rk} + m^{r-1}_{rl}$. Hence, $s^r_{iljk} < s^r_{ijkl} = s^r_{ikjl}$.

Case B2: $m^{r-1}_{jk} < m^{r-1}_{rj} + m^{r-1}_{rk}$ and $m^{r-1}_{jl} \leq m^{r-1}_{rj} + m^{r-1}_{rl}$.

We can assume $m^r_{kl} = m^{r-1}_{kl}$, else we are in *Case B1*, where the roles of points j and k are exchanged. We can also assume $m^{r-1}_{il} < m^{r-1}_{ri} + m^{r-1}_{rl}$. Indeed, if $m^{r-1}_{il} \geq m^{r-1}_{ri} + m^{r-1}_{rl}$ then $s^r_{ijkl} = m^{r-1}_{ri} + s^{r-1}_{rjkl}$, $s^r_{ikjl} = m^{r-1}_{ri} + s^{r-1}_{rkjl}$, and $s^r_{iljk} = m^{r-1}_{ri} + s^{r-1}_{rljk}$ and we are done since $M^{r-1} \in \mathcal{M}_n$.

But now, $s^r_{rlik} > s^r_{rkil}$, and we know from *Case A* that $s^r_{rikl} = s^r_{rlik}$, which means that $m^r_{kl} = m^{r-1}_{rk} + m^{r-1}_{rl}$. Hence, $s^r_{rjkl} > s^r_{rljk}$, and we know from *Case A* that $s^r_{rkjl} = s^r_{rjkl}$, which means that $m^r_{jl} = m^{r-1}_{rj} + m^{r-1}_{rl}$. We therefore have $s^r_{iljk} < s^r_{ijkl} = s^r_{ikjl}$.

Case B3: $m^{r-1}_{jk} \geq m^{r-1}_{rj} + m^{r-1}_{rk}$ and $m^{r-1}_{jl} > m^{r-1}_{rj} + m^{r-1}_{rl}$.

We may assume $m^{r-1}_{il} \geq m^{r-1}_{ri} + m^{r-1}_{rl}$, else the situation is equivalent either to *Case B1* or *B2* (where the roles of points i and j are exchanged, as well as those of k and l) Hence, $s^r_{ijkl} \leq s^r_{ikjl} = s^r_{iljk}$.

Case B4: $m^{r-1}_{jk} \geq m^{r-1}_{rj} + m^{r-1}_{rk}$ and $m^{r-1}_{jl} \leq m^{r-1}_{rj} + m^{r-1}_{rl}$.

Since $M^{r-1} \in \mathcal{M}_n$, and $s^{r-1}_{rijl} < s^{r-1}_{rlij}$ we know that $s^{r-1}_{rjil} = s^{r-1}_{rlij}$, which means that $m^r_{il} < m^{r-1}_{il}$. If $m^{r-1}_{jl} = m^{r-1}_{rj} + m^{r-1}_{rl}$ then $s^r_{ijkl} \leq s^r_{ikjl} = s^r_{iljk}$. Else, $m^{r-1}_{jl} < m^{r-1}_{rj} + m^{r-1}_{rl}$, which implies $s^r_{rkjl} < s^r_{rljk}$. We then know from *Case A* that $s^r_{rjkl} = s^r_{rljk}$, which means that $m^r_{kl} = m^{r-1}_{rk} + m^{r-1}_{rl}$. We therefore have $s^r_{ikjl} < s^r_{ijkl} = s^r_{iljk}$. □

Corollary 1 *Each matrix in $\mathcal{M}_n$ has a unique realization as a tree, and this realization is optimal.*

Proof. Let M be any matrix in $\mathcal{M}_n$, and let $M' = (m'_{ij})$ be the $n \times n$ matrix obtained from M by setting $m'_{ij} = d^{K_M}_{ij}$ for all $1 \leq i < j \leq n$. It follows from Definition 2 that a graph is a realization of M if and only if it is a realization of M'. We know from the above theorem that M' is a tree metric. To conclude, it is sufficient to observe that each tree metric has a unique tree realization, and this realization is optimal. □

3 A related problem

Given two $n \times n$ tree metrics $L = (l_{ij})$ and $U = (u_{ij})$, the *matrix sandwich problem* [3] is to find (if possible) a tree metric $M = (m_{ij})$ such that $l_{ij} \leq m_{ij} \leq u_{ij}$ for all $i \in \{1, \ldots, n\}$. Typically, the information concerning the distance matrix associated with a network may be inaccurate, an we are only given lower and upper bound matrices L and U.

We prove here below that a solution to the matrix sandwich problem can be obtained by first finding a matrix $M \in \mathcal{M}_n$ that lies between L and U, and then constructing the tree metric $M' = (m'_{ij})$ with $m'_{ij} = d_{ij}^{K_M}$. Finding a matrix $M \in \mathcal{M}_n$ that lies between L and U is possibly easier than finding a tree metric with the same lower and upper bound matrices, the reason being that the triangle inequality is not imposed on matrices in $\mathcal{M}_n$.

Proposition 1 *Let $M = (m_{ij})$ be a matrix in $\mathcal{M}_n$, and let $M' = (m'_{ij})$ be the $n \times n$ matrix obtained from M by setting $m'_{ij} = d_{ij}^{K_M}$ for all i and j in $\{1, \ldots, n\}$. If $l_{ij} \le m_{ij} \le u_{ij}$ for all $i \in \{1, \ldots, n\}$, then M' is a solution to the matrix sandwich problem.*

Proof. Let $M = (m_{ij})$ be a matrix in $\mathcal{M}_n$, such that $l_{ij} \le m_{ij} \le u_{ij}$ for all $i \in \{1, \ldots, n\}$. Since L and U are tree metrics, it follows that M has a zero diagonal and positive entries. Let $M' = (m'_{ij})$ be the $n \times n$ matrix obtained from M by setting $m'_{ij} = d_{ij}^{K_M}$ for all $1 \le i < j \le n$. We know from Theorem 1 that M' is a tree metric. Moreover, since L is a tree metric, we have $l_{ij} \le m'_{ij} \le m_{ij}$ for all $i, j \in \{1, \ldots, n\}$. □

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