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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.

Keywords: matrices, tree metrics, 4-point condition.

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Introduction

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

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

By denoting $s_{ijkl} = m_{ij} + m_{kl}$, the 4-point condition is equivalent to imposing that two of the three sums s_{ijkl}, s_{ikjl} and s_{iljk} are equal and not less than the third. 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 [1–3, 7–10].

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It is well known that a tree metric $M = (m_{ij})$ can be represented by an unrooted tree T such that $\{1, \dots, n\}$ is a subset of the vertex set of T, and the length of the unique chain connecting two vertices i and j in T ($1 \le i < j \le n$) 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 0.1. Let M be a symmetric $n \times n$ matrix with zero diagonal and such that $0 \le m_{ij} \le m_{ik} + m_{kj}$ for all i, j, k in $\{1, \dots, n\}$. A graph $G = (V, E, d)$ is a realization of $M = (m_{ij})$ if and only if $\{1, \dots, n\}$ is a subset of V, and $d^G_{ij} = m_{ij}$ for all i, j in $\{1, \dots, n\}$.

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 [7] have proved that tree metrics have a unique realization as a tree, and this realization is optimal. Culberson and Rudnicki [4] have designed an $O(n^2)$ time algorithm for constructing a realization as a tree of tree metrics.

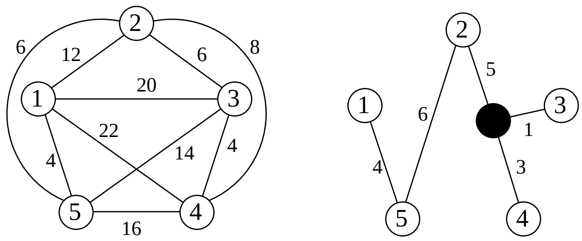
We propose to extend the above definition to matrices whose entries do not necessarily satisfy the triangle inequality. Given a symmetric $n \times n$ matrix $M = (m_{ij})$ with zero diagonal and positive entries, let K_M denote the complete graph on n vertices in which each edge (i, j) has length m_{ij}.

Definition 0.2. 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 $\{1, \dots, n\}$ is a subset of V, and $d^G_{ij} = d^{K_M}_{ij}$ for all i, j in $\{1, \dots, n\}$.

Obviously, if M satisfies the triangle inequality, then $d^{K_M}_{ij} = m_{ij}$, and Definition 0.2 is then equivalent to Definition 0.1. 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.

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

A matrix M.



Its associated complete graph K_M.

A realization of M as a tree.

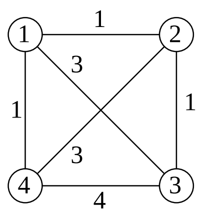
FIGURE 1. a tree realization of a tree metric

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

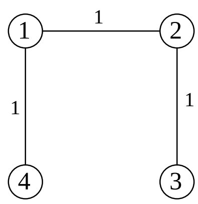
Since we only impose the 4-point condition on *distinct* points i, j, k, l, the entries of a matrix in $\mathcal{M}_n$ do not necessarily satisfy the triangle inequality. While all tree metrics belong to $\mathcal{M}_n$, the example in Figure 2 shows that a matrix having a realization as a tree does 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 $\mathcal{M}_n$

1. 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 $O(n^3)$ time algorithm [6] for the computation of M'.

Floyd's algorithm [6]
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 1.1. *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 $s^r_{ijkl} = m^r_{ij} + m^r_{kl}$. 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 $s^r_{ijkl} \leq max\{s^r_{ikjl}, s^r_{iljk}\}$ for all distinct i, j, k, l in $\{1, \ldots, n\}$, or equivalently, that two of the three sums s^r_{ijkl}, s^r_{ikjl} and s^r_{iljk} are equal and not less than the third.

Notice that $m^r_{ri} = m^{r-1}_{ri}$ and $m^r_{ij} \leq m^{r-1}_{ij}$ 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 (wlog) that $s^{r-1}_{rijk} \leq s^{r-1}_{rjik} = s^{r-1}_{rkij}$. If $m^r_{ik} = m^{r-1}_{ik}$ and $m^r_{ij} = m^{r-1}_{ij}$, then $s^r_{rijk} \leq s^r_{rjik} = s^r_{rkij}$ and we are done. So, we can assume wlog $m^r_{ik} < m^{r-1}_{ik}$. It then follows that $m^{r-1}_{ri} + s^{r-1}_{rjik} = m^{r-1}_{ri} + s^{r-1}_{rkij} < m^{r-1}_{ik} + m^{r-1}_{ij}$, which means that $m^r_{ij} = m^{r-1}_{ri} + m^{r-1}_{rj} < m^{r-1}_{ij}$. We therefore have $s^r_{rijk} \leq m^{r-1}_{ri} + m^{r-1}_{rj} + m^{r-1}_{rk} = s^r_{rjik} = s^r_{rkij}$.

Case B : $r \notin \{i, j, k, l\}$.
If $s^r_{ijkl} = s^{r-1}_{ijkl}, s^r_{ikjl} = s^{r-1}_{ikjl}$ and $s^r_{iljk} = s^{r-1}_{iljk}$, there is nothing to prove. So assume wlog that $m^r_{ij} < m^{r-1}_{ij}$. Notice that if $m^r_{ik} = m^{r-1}_{ik}$, $m^r_{il} = m^{r-1}_{il}$, $m^r_{jk} = m^{r-1}_{jk}$ and $m^r_{jl} = m^{r-1}_{jl}$, then we are done. Indeed, since $M^{r-1} \in \mathcal{M}_n$ and $s^r_{rkij} < s^{r-1}_{rkij}$, while $s^r_{rjik} = s^{r-1}_{rjik}$ and $s^r_{rijk} = s^{r-1}_{rijk}$, we know from Case A that $s^{r-1}_{rjik} = s^{r-1}_{rijk}$. In a similar way, we also have $s^{r-1}_{rjil} = s^{r-1}_{rijl}$. Hence, $s^{r-1}_{rjik} + s^{r-1}_{rijl} = s^{r-1}_{rijk} + s^{r-1}_{rjil}$, which means that $s^{r-1}_{ikjl} = s^{r-1}_{iljk}$. Since $M^{r-1} \in \mathcal{M}_n, s^r_{ikjl} = s^{r-1}_{ikjl}, s^r_{iljk} = s^{r-1}_{iljk}$ and $s^r_{ijkl} < s^{r-1}_{ijkl}$ we conclude that $s^r_{ijkl} < s^r_{ikjl} = s^r_{iljk}$. Wlog, we can therefore assume $m^r_{ik} < m^{r-1}_{ik}$.

The rest of the proof is divided into four subcases.

Case B1 : $m^{r-1}_{jk} < m^{r-1}_{rj} + m^{r-1}_{rk}$ and $m^{r-1}_{jl} > m^{r-1}_{rj} + m^{r-1}_{rl}$.
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 : $m_{jk}^{r-1} \geq m_{rj}^{r-1} + m_{rk}^{r-1}$ and $m_{jl}^{r-1} > m_{rj}^{r-1} + m_{rl}^{r-1}$.
It follows from Cases B1 and B2 that i, j, k and l satisfy the 4-point condition in M^r if $m_{ij}^r < m_{ij}^{r-1}$, $m_{ik}^r < m_{ik}^{r-1}$, and $m_{jk}^{r-1} < m_{rj}^{r-1} + m_{rk}^{r-1}$. By permuting the roles of points i and j as well as those of k and l, we also know that i, j, k and l satisfy the 4-point condition in M^r if $m_{ij}^r < m_{ij}^{r-1}$, $m_{jl}^r < m_{jl}^{r-1}$, and $m_{il}^{r-1} < m_{ri}^{r-1} + m_{rl}^{r-1}$. Since $m_{ij}^r < m_{ij}^{r-1}$ and $m_{jl}^r < m_{jl}^{r-1}$ in Case B3, we can assume $m_{il}^{r-1} \geq m_{ri}^{r-1} + m_{rl}^{r-1}$. Hence, $s_{ijkl}^r \leq s_{ikjl}^r = s_{iljk}^r$.

Case B4 : $m_{jk}^{r-1} \geq m_{rj}^{r-1} + m_{rk}^{r-1}$ and $m_{jl}^{r-1} \leq m_{rj}^{r-1} + m_{rl}^{r-1}$.
Since $M^{r-1} \in \mathcal{M}_n$, and $s_{rijl}^{r-1} < s_{rlij}^{r-1}$ we know that $s_{rjil}^{r-1} = s_{rlij}^{r-1}$, which means that $m_{il}^r < m_{il}^{r-1}$. If $m_{jl}^{r-1} = m_{rj}^{r-1} + m_{rl}^{r-1}$ then $s_{ijkl}^r \leq s_{ikjl}^r = s_{iljk}^r$. Else, $m_{jl}^{r-1} < m_{rj}^{r-1} + m_{rl}^{r-1}$, which implies $s_{rkjl}^r < s_{rljk}^r$. We then know from Case A that $s_{rjkl}^r = s_{rljk}^r$, which means that $m_{kl}^r = m_{rk}^{r-1} + m_{rl}^{r-1}$. We therefore have $s_{ikjl}^r < s_{ijkl}^r = s_{iljk}^r$.

□

Corollary 1.2. *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 $m'_{ij} = d_{ij}^{K_M}$ for all $1 \leq i < j \leq n$. It follows from Definition 0.2 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. □

2. A related problem

Given two $n \times n$ metrics $L = (l_{ij})$ and $U = (u_{ij})$, the *matrix sandwich problem* [5] is to find (if possible) a tree metric $M = (m_{ij})$ such that $l_{ij} \leq m_{ij} \leq u_{ij}$ for all $i, j \in \{1, \ldots, n\}$. Typically, the information concerning the distance matrix associated with a network may be inaccurate, and 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 2.1. *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 $l_{ij} \leq m_{ij} \leq u_{ij}$ for all $i, j \in \{1, \ldots, n\}$, 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 $i, j \in \{1, \dots, n\}$, and let $M' = (m'_{ij})$ be the $n \times n$ matrix obtained from M by setting $m'_{ij} = d^{K_M}_{ij}$ for all $1 \le i < j \le n$. We know from Theorem 1 that M' is a tree metric. Moreover, since L is a metric, we have $l_{ij} \le m'_{ij} \le m_{ij}$ for all $i, j \in \{1, \dots, n\}$. $\square$

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