

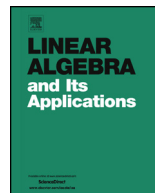


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## Potentials of random walks on trees



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### ABSTRACT

In this article we characterize inverse  $M$ -matrices and potentials whose inverses are supported on trees. In the symmetric case we show they are a Hadamard product of tree ultrametric matrices, generalizing a result by Gantmacher and Krein [12] done for inverse tridiagonal matrices. We also provide an algorithm that recognizes when a positive matrix  $W$  has an inverse  $M$ -matrix supported on a tree. This algorithm has quadratic complexity. We also provide a formula to compute  $W^{-1}$ , which can be implemented with a linear complexity. Finally, we also study some stability properties for Hadamard products and powers.

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## 1. Introduction and basic definitions

Markov chains are used to model a variety of phenomena and one is accustomed to estimate its transition probability  $P$  in order to simulate and understand the underline probabilistic structure. Nevertheless, there are some situations where a direct measurement of  $P$  is not available. For example, this happens in electrical networks, where  $P$  is

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related to the resistances of the network (see for example [10] section 2.7). Instead, we can measure the potential  $W$  of the Markov chain, which is the mean expected number of visits per site (assuming the chain is transient). These two matrices are related by  $W = (\mathbb{I} - P)^{-1}$ , so in principle one can model  $W$  instead of  $P$ . The main drawback of this approach is that structural restrictions for potentials are difficult to state (this is part of the inverse  $M$ -matrix problem).

In this article, we show how to handle this problem under the extra hypothesis that the incidence graph of  $W^{-1}$  is a tree. In the nomenclature of Klein [15],  $W^{-1}$  is a **treediagonal**. This is the case of a linear tree like Birth and Death chains and some networks like the electric power distribution system. In [Theorem 2.5](#), we show that to reconstruct the chain it is enough to measure the potential at edges and nodes of the tree. The unique restrictions on those numbers are given by the  $2 \times 2$  determinants associated with every edge. On the other hand, [Theorem 2.2](#) (see also [Corollary 2.3](#)) provides an explicit formula to compute  $P$  from  $W$ . The complexity of this formula is linear in the number of nodes in the tree. More explicitly, if  $W$  is an  $n \times n$  matrix, then the algorithm obtained from this formula, uses at most  $11n$  operations (products, divisions and sums) to compute  $W^{-1}$ . Notice here that while  $W^{-1}$  is a sparse matrix,  $W$  itself is a full matrix (under irreducibility  $W > 0$ ).

For the sake of completeness, we recall that a matrix  $Q$  is an  **$M$ -matrix** if it is a  $Z$ -matrix, that is, the off diagonal elements are nonpositive,  $Q$  is nonsingular and the entries of its inverse  $Q^{-1}$  are nonnegative. We refer to [13] section 2.5 for a set of equivalent conditions that characterize  $M$ -matrices. It is worth mentioning that the diagonal entries of an  $M$ -matrix are positive. On the other hand, a relevant sufficient condition for a  $Z$ -matrix  $Q$  to be an  $M$ -matrix, is that  $Q$  is nonsingular and **row diagonally dominant**, that is, for all  $i$  the row sum  $\sum_j Q_{ij} \geq 0$ .

In [Theorem 2.7](#) we characterize, in an algorithmic way, those positive matrices whose inverses are  $M$ -matrices supported on a tree. The associated algorithm is developed in [Appendix B](#), which provides the tree associated with  $W^{-1}$  with a complexity bounded by  $\frac{37}{2}n^2$ .

As a complement, [Theorem 2.1](#) provides a description of a potential associated with a Markov chain supported on a tree. This is done in terms of ultrametric matrices. A sufficient condition is that  $U = \text{diag}(1./W_{\bullet r}) W \text{diag}(1./W_{r \bullet})$  is an ultrametric matrix. On the other hand, in the symmetric case, a necessary and sufficient condition is that  $W$  is the Hadamard product of tree ultrametric matrices, plus condition (2.2). As tree ultrametric matrices are simple to construct, this result provides a simple way to describe general Markov chains on trees.

In [9], we have proved that every potential of a random walk on  $\{1, \dots, n\}$  with nearest neighbor transitions, is the product of a positive diagonal matrix with a matrix which is the Hadamard product of two ultrametric matrices. This is equivalent to representing the inverse of a tridiagonal and row diagonally dominant  $M$ -matrix as such product. This was done in the symmetric case in [12]. In our setting, we shall see that we require one ultrametric matrix per extremal point of the set (on the tree) where the chain is losing

mass. This explains why for nearest neighbor random walks, we needed two ultrametric matrices (in some simple cases we needed just one).

Finally, in [Theorem 2.8](#) we study stability properties for these matrices under Hadamard products and powers. In particular we show that if  $W, Z$  are two inverse treediagonal  $M$ -matrices associated with the same tree  $\mathbb{T}$ , then their Hadamard product  $W \odot Z$  is also an inverse treediagonal  $M$ -matrix associated with  $\mathbb{T}$ .

To continue, let us recall the definition of a potential matrix.

**Definition 1.1.** A nonnegative and nonsingular matrix  $W$  is said to be a **potential** if  $M = W^{-1}$  is a row diagonally dominant  $M$ -matrix.

The inverse of a potential matrix  $W$  is a row diagonally dominant  $M$ -matrix, so there exist a transient substochastic matrix  $P$  and a constant  $k$  such that  $W^{-1} = k(\mathbb{I} - P)$ . In particular,  $W$  is proportional to the potential (in the probabilistic sense) of the Markov chain associated with  $P$ , which is  $U = (\mathbb{I} - P)^{-1}$ . This matrix represents the expected number of visits for this Markov chain. Indeed, since  $P$  is transient, the series  $\sum_{m \geq 0} P^m$  is finite and  $U = (\mathbb{I} - P)^{-1} = \sum_{m \geq 0} P^m$ . Hence, if we consider  $(X_n)$  a Markov chain whose transition kernel is  $P$  then

$$U_{ij} = \sum_n P_{ij}^n = \sum_n \mathbb{E}_i(\mathbb{1}_j(X_n)) = \mathbb{E}_i \left( \sum_n \mathbb{1}_j(X_n) \right),$$

where  $\mathbb{E}_i$  is the mean expected value when the starting condition is  $X_0 = i$ , and  $\mathbb{1}_j(x)$  is the function that takes the value 1 when  $x = j$  and 0 otherwise.

Since  $U$  and  $W$  are proportional we conclude that for all  $i \neq j$

$$W_{ij} = f_{ij}^W W_{jj}, \tag{1.1}$$

where  $f_{ij}^W \in [0, 1]$  is the probability that the chain ever visits  $j$  starting from  $i$ . This quantity can be described using the hitting time  $\tau_j = \inf\{n \geq 0 : X_n = j\}$ , which is the first random time the chain visits  $j$  (we put  $\tau_j = \infty$  for those realizations where the chain never visits  $j$ ). Then,

$$f_{ij}^W = \mathbb{P}_i(\tau_j < \infty).$$

In the sequel we define  $f_{ii}^W = 1$ , in order that [\(1.1\)](#) is satisfied for all  $i, j$ .

In particular if  $W$  is a potential, then  $W$  is column pointwise diagonally dominant, that is for all  $i, j$

$$W_{ij} \leq W_{jj}.$$

If  $W$  is symmetric, we get it is also row pointwise diagonally dominant. Also, we point out that  $W > 0$  if and only if the associated chain is irreducible, or equivalently, the incidence graph of  $W^{-1}$  is connected.

**Remark 1.1.** There is a subtle difference between  $W$  being a potential and  $W^{-1} = \mathbb{I} - P$ , for some substochastic matrix  $P$ . Of course the latter is a special case of the former. To give a probabilistic representation of a general potential matrix, one has to use a continuous time Markov chain  $X = (X_t : t \in \mathbb{R}^+)$ . This process is like a Markov chain but jumps from one site to another after certain exponentially distributed random times. Again,  $W_{ij}$  represents the mean total time spent by  $X$  at site  $j$ , starting from  $i$  (see [10] Section 2.3.1).

Recall that a graph  $\mathbb{G} = (\mathcal{V}, \mathcal{E})$  is a set of vertices or nodes  $\mathcal{V}$  and a set of edges  $\mathcal{E} \subset \mathcal{V} \times \mathcal{V}$ . When there is no possible confusion we shall not distinguish between  $i \in \mathbb{G}$  and  $i \in \mathcal{V}$ . Also, we shall not distinguish between  $(i, j) \in \mathbb{G}$  and  $(i, j) \in \mathcal{E}$ .

**Definition 1.2.** Given an  $M$ -matrix  $M$  with inverse  $W$ , the graph  $\mathbb{G} = \mathbb{G}(W)$ , denotes the incidence graph of  $M$ , that is,  $(i, j) \in \mathbb{G}$  if and only if  $M_{ij} \neq 0$ . We shall say that  $\mathbb{G}$  is the graph associated with  $W$  (and  $M$ ).

On the other hand, we say that a node  $i$  is a **root** of  $W$  (or  $M$ ) if  $\sum_j M_{ij} \neq 0$ . The set of roots of  $W$  is denoted by  $\mathcal{R}(W)$ .

The unique solution to  $W\mu = \mathbb{1}$ , that is  $\mu = M\mathbb{1}$ , is called the **right signed equilibrium potential** of  $W$  and it will be denoted by  $\mu_W$ . The support of  $\mu_W$  is the set of nodes  $\{i : (\mu_W)_i \neq 0\}$ , which is exactly the set of roots for  $W$ . The total mass of  $\mu_W$  is denoted by  $\bar{\mu}_W = \mu'_W \mathbb{1}$ .

Since the diagonal elements of an  $M$ -matrix are positive  $\mathbb{G}(W)$  always contains the loop  $(i, i)$  for all  $i \in \mathcal{V}$ . Also, we point out that in principle  $\mathbb{G}(W)$  is a directed graph. Nevertheless, we shall consider mainly the case where  $\mathbb{T} = \mathbb{G}(W)$  is a tree. In particular  $(i, j) \in \mathbb{T}$  means that both  $W_{ij}^{-1} \neq 0$  and  $W_{ji}^{-1} \neq 0$ . This is slightly different from what is done in [15] or [19], where the graph considered is defined as  $(i, j) \in \mathbb{G}(W^{-1})$  if and only if  $W_{ij}^{-1} \neq 0$  or  $W_{ji}^{-1} \neq 0$ . However, if  $\mathbb{G}(W)$  is a tree and  $W^{-1}$  is irreducible (or equivalently  $W > 0$ ) both concepts coincide.

If  $(\mu_W)_i \geq 0$  then  $M$  is row diagonally dominant at row  $i$ . Hence, the right signed equilibrium measure  $\mu_W$  is nonnegative if and only if  $W^{-1}$  is row diagonally dominant. In this case we say that  $\mu_W$  is the **right equilibrium potential** of  $W$ .

We point out that when  $W$  is a potential the decomposition of  $W^{-1} = k(\mathbb{I} - P)$  is not unique, but the connections determined by  $P$  out of the diagonal are well defined:  $i \neq j$  are connected in one step, that is  $P_{ij} > 0$ , if and only if  $(i, j) \in \mathbb{G}(W)$ . Thus  $\mathbb{G}(W)$  represents the graph of transitions for the underline Markov chain. We notice that  $i$  is a root (as defined before) if  $P$  is defective at  $i$ , that is

$$\sum_j P_{ij} < 1. \tag{1.2}$$

Hence, the Markov chain loses mass exactly at the roots of  $W$ .

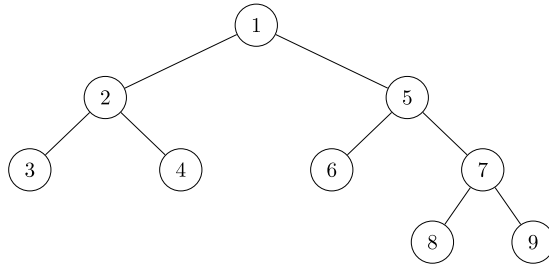


Fig. 1. A tree  $\mathbb{T}$  and a subset  $\mathcal{A}$ .

A tree  $\mathbb{T} = (\mathcal{V}, \mathcal{E})$  is a non-oriented, connected graph without simple cycles. Unless we say the contrary, we assume that for every  $i \in \mathcal{V}$  the loop  $(i, i) \in \mathcal{E}$ . In what follows  $\mathbb{T}$  will denote indistinctly the tree, the set of nodes and the set of arcs, unless it is necessary to do the distinction.

For a pair of different nodes  $i, j \in \mathbb{T}$  we can distinguish a particular path that joins these two points. Namely, the geodesic between  $i$  and  $j$ , which is the shortest path in  $\mathbb{T}$  that connects them. We denote by  $geod_{\mathbb{T}}(i, j)$  this path, which is characterized by  $geod_{\mathbb{T}}(i, j) = \{i_0 = i, \dots, i_p = j\}$  where all nodes are different and two consecutive nodes are neighbors in  $\mathbb{T}$ . The length of this path is denoted by  $d_{\mathbb{T}}(i, j) = p$ . By convention we assume  $geod_{\mathbb{T}}(i, i) = \{i\}$  and  $d_{\mathbb{T}}(i, i) = 0$ . A node  $i \in \mathbb{T}$  is called a **leaf** if it has a unique (immediate) neighbor in  $\mathbb{T}$ , that is, a unique  $j \in \mathbb{T}$  such that  $d_{\mathbb{T}}(i, j) = 1$ . The set of leaves of  $\mathbb{T}$  is denoted by  $\mathcal{L}(\mathbb{T})$ . Notice that if  $\mathbb{T}$  has exactly two leaves then it is a path (a linear tree).

We also denote  $i \sim j$  to mean that  $i \neq j$  and  $(i, j) \in \mathbb{T}$  or equivalently that  $d_{\mathbb{T}}(i, j) = 1$ .

We shall need the following concept

**Definition 1.3.** Given a set  $\mathcal{A} \subset \mathbb{T}$ , we say that  $i \in \mathcal{A}$  is **extremal** in  $\mathcal{A}$  if

$$\forall k, l \in \mathcal{A}, i \in geod_{\mathbb{T}}(k, l) \Rightarrow [i = k \text{ or } i = l].$$

We denote by  $ext(\mathcal{A})$  the set of extremal points of  $\mathcal{A}$ . We also denote by  $\mathbb{T}(\mathcal{A})$  the smallest subtree of  $\mathbb{T}$  that contains  $\mathcal{A}$  and we call it the **tree generated by  $\mathcal{A}$** .

Notice that  $\mathbb{T}(ext(\mathcal{A})) = \mathbb{T}(\mathcal{A})$ ,  $ext(\mathbb{T}(\mathcal{A})) = ext(\mathcal{A})$  and  $ext(\mathbb{T}) = \mathcal{L}(\mathbb{T})$ .

**Example 1.1.** Consider the tree given in Fig. 1 and  $\mathcal{A} = \{2, 4, 5, 6, 7, 8\}$ .

Then,  $ext(\mathcal{A}) = \{4, 6, 8\}$  and  $\mathbb{T}(\mathcal{A}) = \{1, 2, 4, 5, 6, 7, 8\}$ .

Another important concept for this article is the notion of ultrametric matrix, which we recall in the next definition (see [16]).

**Definition 1.4.** A symmetric nonnegative matrix  $U$  is **ultrametric** if for all  $i, j, k$  we have

$$U_{ij} \geq \min\{U_{ik}, U_{kj}\}.$$

In particular, if  $i = j$  we obtain that

$$U_{ii} \geq \max\{U_{ik} : k \in I, k \neq i\}$$

If this last inequality is strict for all  $i$  then  $U$  is said to be **strictly ultrametric**.

## 2. Main results

In this section we establish the main results of this article. Some of them require a precise study of ultrametric matrices on trees, which we postpone to the next section. We shall see there are two types of them. What we call class 1 (see Definition 3.2) are the ones that have a unique root, that is, a unique node where the associated Markov chain is losing mass.

**Theorem 2.1.** *Assume that  $W$  is an inverse  $M$ -matrix, whose graph  $\mathbb{T} = \mathbb{G}(W)$  is a tree. Then:*

- (i) *There exist diagonal matrices  $F, E$  such that  $FW$  is a potential,  $WE$  is a symmetric inverse  $M$ -matrix and furthermore we can choose them such that  $FWE$  is a symmetric potential. Since  $F, E$  are diagonal matrices then  $\mathbb{T}$  is the graph associated with  $FW, EW, FWE$ . If  $W$  is symmetric we can take  $E = F$ . On the other hand, if  $W$  is a potential we can take  $F = \mathbb{I}$ .*
- (ii) *For any node  $r \in \mathbb{T}$  the matrix*

$$U = \text{diag}(1./W_{\bullet,r}) W \text{diag}(1./W_{r,\bullet})$$

*is a class 1 tree ultrametric matrix such that  $\mathbb{T} = \mathbb{G}(U)$  and whose unique root is  $r$ ;*

- (iii) *Assume now  $W$  is a symmetric potential with set of roots  $\mathcal{R}(W)$ . For every  $\ell \in \text{ext}(\mathcal{R}(W))$  there exists a nonsingular class 1 tree ultrametric matrix  $U_\ell$  with  $\mathbb{T} = \mathbb{G}(U_\ell)$  and a unique root at  $\ell$ , such that*

$$W = \bigoplus_{\ell \in \text{ext}(\mathcal{R}(W))} U_\ell.$$

*That is,  $W$  is the Hadamard product of class 1 tree ultrametric matrices.*

The decomposition given in (iii) bears some similarities with the decomposition given in Theorem 3.4 [19] (see also this article for further references, in particular the works [11] and [14]). We notice that in the case of a linear tree, that is  $W^{-1}$  is a tridiagonal matrix then the result was shown in [12] (see [18,19,9]).

As a sort of converse we have the following result, in which we also provide a formula for  $W^{-1}$  in terms of the entries of  $W$ .

**Theorem 2.2.** Assume  $\mathbb{T}$  is a tree and  $\mathcal{A} \subset \mathbb{T}$ . Take for every  $\ell \in \mathcal{A}$  a nonsingular class 1 tree ultrametric matrix  $U_\ell$  with root at  $\ell$  and  $\mathbb{G}(U_\ell) = \mathbb{T}$ . Then,

- (i)  $W = \bigodot_{\ell \in \mathcal{A}} U_\ell$  is a symmetric inverse  $M$ -matrix and  $\mathbb{G}(W) = \mathbb{T}$ .
- (ii) For every  $t \notin \mathbb{T}(\mathcal{A})$  the corresponding row sum of  $W^{-1}$  is 0 and for every  $t \in \text{ext}(\mathcal{A})$  the row sum is strictly positive. Therefore, we have the relation

$$\text{ext}(\mathcal{A}) \subset \mathcal{R}(W) \subset \mathbb{T}(\mathcal{A})$$

and  $\text{ext}(\mathcal{R}(W)) = \text{ext}(\mathcal{A})$ .

- (iii)  $W^{-1}$  is given by the formula

$$\begin{aligned} W_{ii}^{-1} &= \frac{1}{W_{ii}} \left( 1 + \sum_{t: d_{\mathbb{T}}(i,t)=1} \frac{W_{it}W_{ti}}{W_{tt}W_{ii} - W_{it}W_{ti}} \right), \\ W_{ij}^{-1} &= -\frac{W_{ij}}{W_{jj}W_{ii} - W_{ij}W_{ji}}, \text{ if } d_{\mathbb{T}}(i,j) = 1, \\ W_{ij}^{-1} &= 0, \text{ if } d_{\mathbb{T}}(i,j) > 1. \end{aligned} \tag{2.1}$$

- (iv) A necessary and sufficient condition for  $W$  to be a potential is that  $W|_{\mathbb{T}(\mathcal{A})}$  is a potential. Using (2.1) this is equivalent to having for all  $i$

$$\frac{1}{W_{ii}} \geq \sum_{t: d_{\mathbb{T}}(i,t)=1} \frac{W_{it}}{W_{tt}W_{ii} - W_{it}W_{ti}} \left( 1 - \frac{W_{ti}}{W_{ii}} \right). \tag{2.2}$$

Moreover, the roots of  $W$  are those nodes  $i \in I$ , for which there is strict inequality in (2.2).

**Remark 2.1.** Ultrametric matrices are pointwise diagonally dominant. So, if  $W$  is the Hadamard product of ultrametric matrices, then  $W$  is also pointwise diagonally dominant. This shows that the right hand side of (2.2) is nonnegative. Also notice that we have stated formula (2.1) and condition (2.2) as if  $W$  is not symmetric. We have done it in this way because they extend to the case where  $W$  is not symmetric.

**Remark 2.2.** The decomposition given in Theorem 2.1 (iii) (or Theorem 2.2 (i)) could be used to simulate symmetric inverse  $M$ -matrices whose associated graphs are trees. In fact, consider  $\mathbb{T}$  a tree,  $\mathcal{A} \subset \mathbb{T}$  and simulate for every  $\ell \in \mathcal{A}$  an ultrametric matrix  $U_\ell$ , whose inverse is supported on  $\mathbb{T}$  and has a unique root at  $\ell$ . This is done efficiently because ultrametric matrices require only a set of weights that are increasing in the rooted tree  $(\mathbb{T}, \ell)$  (see Section 3). Then, multiply these matrices in the sense of Hadamard, which is a simple matrix operation, to obtain the desired inverse  $M$ -matrix. From the theoretical point of view, this decomposition allows us to show that the Hadamard product of inverse  $M$ -matrices, whose associated graphs are the same tree, is again an inverse  $M$ -matrix

(see Theorem 2.8 (iv)). This is an interesting fact because on the one hand there are not very many known algebraic stability properties for inverse  $M$ -matrices or potentials, and on the other hand the Hadamard product of inverse  $M$ -matrices is not in general an inverse  $M$ -matrix.

Formula (2.1) is an extension of (3.1) and (3.4) (below), which cover the case of a tree ultrametric matrix. This type of formula also appeared in [1] and [19]. In the ultrametric case there is a simple probabilistic proof of it, see Remark 3.2. This together with the representation given in Theorem 2.1 (ii) provides a probabilistic insight of the algebraic identity (2.1).

Using Theorem 2.1 (i) and (2.1), we obtain a formula for the inverse of an  $M$ -matrix supported on a tree (we generalize this corollary in Section 6, Lemma 6.2).

**Corollary 2.3.** *Assume that  $W = M^{-1}$  where  $M$  is an  $M$ -matrix whose incidence graph is the tree  $\mathbb{T}$ . Then*

$$\begin{cases} W_{ii}^{-1} = \frac{1}{W_{ii}} \left( 1 + \sum_{t:d_{\mathbb{T}}(i,t)=1} \frac{W_{it}W_{ti}}{W_{tt}W_{ii} - W_{it}W_{ti}} \right), \\ W_{ij}^{-1} = -\frac{W_{ij}}{W_{jj}W_{ii} - W_{ij}W_{ji}}, \text{ if } d_{\mathbb{T}}(i, j) = 1, \\ W_{ij}^{-1} = 0, \text{ if } d_{\mathbb{T}}(i, j) > 1. \end{cases} \tag{2.3}$$

The following results will give conditions for a positive matrix  $W$  to be an inverse  $M$ -matrix such that  $\mathbb{G}(W)$  is a tree.

**Theorem 2.4.** *Assume that  $A$  is a nonsingular positive matrix, such that the incidence graph of its inverse  $\mathbb{T} = \mathbb{G}(A)$  is a tree. Then, the following are equivalent*

- (i)  $A^{-1}$  is an  $M$ -matrix;
- (ii)  $A_{ii}A_{jj} - A_{ij}A_{ji} > 0$  for all  $i \neq j$ ;
- (iii)  $A_{ii}A_{jj} - A_{ij}A_{ji} > 0$  for all  $i, j$  such that  $d_{\mathbb{T}}(i, j) = 1$ ;

*Under any of these equivalent conditions,  $A$  is a potential if and only if (2.2) holds, that is for all  $i$*

$$\frac{1}{A_{ii}} \geq \sum_{t:d_{\mathbb{T}}(i,t)=1} \frac{A_{it}}{A_{tt}A_{ii} - A_{it}A_{ti}} \left( 1 - \frac{A_{ti}}{A_{ii}} \right).$$

The main characterization of inverse  $M$ -matrices and potentials whose associated graph is a tree, is given by the next result.

**Theorem 2.5.** *Assume that  $\mathbb{T}$  is a tree. To every edge  $(i, j) \in \mathbb{T}, i \neq j$ , we associate two positive numbers  $X_{ij}, X_{ji}$ . To every node  $i \in \mathbb{T}$  we also associate a positive number  $X_{ii}$ .*



We assume that the  $2 \times 2$  determinant  $X_{ii}X_{jj} - X_{ij}X_{ji}$  is positive, for all  $i \neq j$  such that  $(i, j) \in \mathbb{T}$ . Consider the matrix defined by

$$W_{ik} = \begin{cases} X_{ii} & \text{if } i = k \\ X_{ik} & \text{if } i \neq k, (i, k) \in \mathbb{T} \\ \left( \prod_{p=1}^{q-1} \frac{X_{i_{p-1}i_p}}{X_{i_p i_p}} \right) X_{i_{q-1}k} & \text{otherwise,} \end{cases} \tag{2.4}$$

where in the last case  $\text{geod}_{\mathbb{T}}(i, k) = \{i = i_0 \sim i_1 \sim \dots \sim i_{q-1} \sim i_q = k\}$  and  $q \geq 2$ .

Then,  $W$  is an inverse  $M$ -matrix and  $\mathbb{G}(W) = \mathbb{T}$ . Moreover,  $W$  is a potential if and only if (2.2) holds, namely, for all  $i$

$$\frac{1}{X_{ii}} \geq \sum_{t:t \sim i} \frac{X_{it}}{X_{tt}X_{ii} - X_{it}X_{ti}} \left( 1 - \frac{X_{ti}}{X_{ii}} \right).$$

Conversely, assume that  $W$  is an inverse  $M$ -matrix and its associated graph  $\mathbb{T} = \mathbb{G}(W)$  is a tree. Then, all the  $2 \times 2$  principal minors of  $W$  are positive and  $W$  satisfies (2.4) for all  $i, k \in \mathbb{T}$ , where  $X_{ii} = W_{ii}$  and  $X_{ij} = W_{ij}$ , whenever  $d_{\mathbb{T}}(i, j) = 1$ .

The main assumption of the last two theorems is that we know in advance the tree  $\mathbb{T}$ . In Section 7, we study an algorithm that produces this tree directly from the matrix  $W$  (see also Appendix B). The main technical tool to analyze this algorithm is given in Lemma 7.2. This is done in terms of the symmetric matrix  $R = R(W)$  defined as  $R_{ij} = \frac{W_{ij}W_{ji}}{W_{ii}W_{jj}}$ . If  $W$  is a potential of a random walk on a tree, then  $R_{ij}$  represents the probability that starting from  $i$  the chain returns to  $i$  after visiting  $j$ :  $R_{ij} = \mathbb{P}_i(\tau_j < \infty)\mathbb{P}_j(\tau_i < \infty)$  (this quantity is symmetric in  $i, j$ ). Roughly speaking two nodes  $i \neq j$  are neighbors in  $\mathbb{T}$  if this quantity is large

$$R_{ij} > \max\{R_{ik}R_{kj} : k \neq i, j\}.$$

**Definition 2.6.** Consider a positive matrix  $W$  and denote  $R = R(W)$ . For  $i \neq j$  we denote  $i \overset{W}{\sim} j$  whenever  $R_{ij} > \max\{R_{ik}R_{kj}; k \neq i, j\}$ .

The next result is the basis of the algorithm we propose.

**Theorem 2.7.** Assume  $W$  is a positive matrix and let  $R = R(W)$ . We also assume that every  $2 \times 2$  principal minor of  $W$  is positive. The matrix  $W$  is an inverse  $M$ -matrix and  $\mathbb{G}(W)$  is a tree if and only if

- (i) for all  $i$  there exists  $j$  such that  $i \overset{W}{\sim} j$ ;
- (ii) if  $i \overset{W}{\sim} j$  and if we denote  $K = \{k : R_{ki} > R_{kj}\}$ ,  $J = K^c$ , then

$$W_{KJ} = W_{K^i} \frac{W_{ij}}{W_{ii}W_{jj}} W_{jJ}, \quad W_{JK} = W_{Jj} \frac{W_{ji}}{W_{ii}W_{jj}} W_{iK}.$$

Moreover, the tree  $\mathbb{T} = \mathbb{G}(W)$  is given by the relation  $\overset{W}{\sim}$ , that is, for  $i \neq j$  we have

$$(i, j) \in \mathbb{T} \Leftrightarrow i \overset{W}{\sim} j.$$

The next result is devoted to some stability properties of inverse treediagonal  $M$ -matrices under Hadamard powers and products. Recall that for  $\alpha \geq 1$ , the Hadamard power  $W^{(\alpha)}$  of an inverse  $M$ -matrix is always an inverse  $M$ -matrix. This was shown in [2,3,6] (see also [7] for some generalizations). As was shown in Theorem 2.9 in [9], in the case of inverse tridiagonal  $M$ -matrices, this result is also true when  $\alpha > 0$ .

**Theorem 2.8.** *Assume  $W$  is an inverse  $M$ -matrix, with order  $n$ , whose associated graph  $\mathbb{T} = \mathbb{G}(W)$  is a tree.*

- (i) *For all  $\alpha > 0$ , the Hadamard power  $W^{(\alpha)}$  is also an inverse  $M$ -matrix whose graph is the same tree  $\mathbb{T}$ .*
- (ii) *For  $\alpha < 0$ , the matrix  $W^{(\alpha)}$  is nonsingular, its inverse  $C = C(\alpha)$  is supported on  $\mathbb{T}$  and the following properties hold*
  - (ii.1)  *$\text{sign}(\det(W^{(\alpha)})) = (-1)^{n+1}$ ;*
  - (ii.2) *if  $n \geq 2$ , then for all  $i, j$  we have*

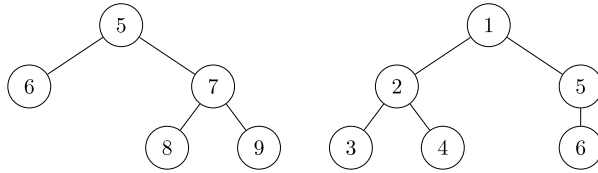
$$C_{ij} \text{ is } \begin{cases} < 0 & \text{if } i = j \\ > 0 & \text{if } d_{\mathbb{T}}(i, j) = 1 ; \\ = 0 & \text{otherwise} \end{cases}$$

- (ii.3) *If  $W$  is symmetric then the eigenvalues of  $W^{(\alpha)}$  are negative, except for the principal one  $\lambda_1$  which is positive and with maximal absolute value.*
- (iii) *Also, if  $\alpha \geq 1$  and  $W$  is a potential, then  $W^{(\alpha)}$  is also a potential. Even more, if  $W^{-1} = \mathbb{I} - P$  for some substochastic kernel supported on  $\mathbb{T}$ , then  $(W^{(\alpha)})^{-1} = \mathbb{I} - Q(\alpha)$  for some substochastic kernel  $Q(\alpha)$  also supported on  $\mathbb{T}$ .*
- (iv) *Finally, if  $Z$  is another inverse  $M$ -matrix such that  $\mathbb{G}(Z) = \mathbb{T}$ , then  $W \odot Z$  is an inverse  $M$ -matrix for which  $\mathbb{G}(W \odot Z) = \mathbb{T}$ .*

### 3. Ultrametric matrices on trees

In this section we summarize and complete the known results about ultrametric matrices that are (proportional to) potentials of Markov chains on trees. We shall see there are two types of such ultrametric matrices, according to whether the associated Markov chain has one or two roots (see also [17] and [19]).

Given a tree  $\mathbb{T}$  and a node  $r \in \mathbb{T}$ , the height of  $i \in \mathbb{T}$  is denoted as  $h_r(i) = d_{\mathbb{T}}(i, r)$  and the height of  $\mathbb{T}$  is defined as  $\mathbf{H}_r = \max\{h_r(i) : i \in \mathbb{T}\}$ . For  $i \in \mathbb{T}$  we denote by  $S_r(i) = \{j \in \mathbb{T} : (i, j) \in \mathbb{T}, h_r(j) = h_r(i) + 1\}$  the set of immediate descendants of  $i$ . For a node  $i \neq r$  we denote by  $i^-$  the unique node in  $\text{geod}_{\mathbb{T}}(i, r)$  such that  $i \in S_r(i^-)$ . Notice that the leaves of  $\mathbb{T}$ , with the exception probably of  $r$ , are those nodes  $i \in \mathbb{T}$  for which  $S_r(i) = \emptyset$ .



**Fig. 2.** The subtree of  $\mathbb{T}$ , in [Example 1.1](#), that hangs from 5 as seen from 1 on the left and as seen from 7 on the right.

Given a node  $v \in \mathcal{V}$  we denote by  $\mathbb{T}_r[v]$  the tree that hangs from  $v$  as seen from  $r$ , which is the subtree of  $\mathbb{T}$  on the set of nodes  $\{i \in \mathcal{V} : v \in \text{geod}_{\mathbb{T}}(i, r)\}$ . We point out that  $\mathbb{T}_r[r] = \mathbb{T}$ . Finally, given two nodes  $i, j$  in  $\mathbb{T}$  we define by  $i \overset{r}{\wedge} j$  the unique point in  $\text{geod}_{\mathbb{T}}(i, r) \cap \text{geod}_{\mathbb{T}}(j, r)$  which has maximal height (w.r.t.  $r$ ). Notice that  $i \overset{r}{\wedge} i = i$  and  $i \overset{r}{\wedge} r = r$ . Also notice that  $\mathbb{T}_r[i \overset{r}{\wedge} j]$  is a subtree of  $\mathbb{T}$  that contains both  $i, j$  (and it is the minimal subtree in some sense with this property). We point out that  $h_r(\bullet), \mathbf{H}_r, S_r(\bullet), \mathbb{T}_r[\bullet]$  and  $\overset{r}{\wedge}$  depend on  $r$  (see [Fig. 2](#)).

Recall that in the language of graph Theory  $r$  is called also a root, which is quite different from the concept we have considered above. While in some cases both concepts will agree they are not necessarily the same. To emphasize the difference, when it is needed, we shall refer to  $r$  as a probabilistic root when it satisfies [\(1.2\)](#), that is  $r \in \mathcal{R}(W)$ .

In the next results we shall characterize the class of ultrametric matrices that are potential matrices of random walks on trees. To describe this class we need the following definitions.

**Definition 3.1.** Assume that  $\mathbb{T} = (\mathcal{V}, \mathcal{E})$  is a tree and  $r \in \mathcal{V}$  is a fixed node. A real function  $F : \mathcal{A} \subset \mathcal{V} \rightarrow \mathbb{R}$  is said to be  **$r$ -increasing** if for all  $i, j \in \mathcal{A}$  such that  $i \in \text{geod}_{\mathbb{T}}(j, r)$  then  $F(i) \leq F(j)$ .

An  $r$ -increasing function  $F$  is an increasing function on each branch of  $\mathbb{T}$  as seen hanging from  $r$ .

**Definition 3.2.** Consider:

- A tree  $\mathbb{T} = (\mathcal{V}, \mathcal{E})$  and nodes  $r, s \in \mathcal{V}$ , not necessarily different, such that  $(r, s) \in \mathcal{E}$  (recall that loops are allowed edges);
- A function  $F : \mathcal{V} \rightarrow \mathbb{R}_+$  such that  $F|_{\mathbb{T}_s[r]}$  is  $r$ -increasing and  $F|_{\mathbb{T}_r[s]}$  is  $s$ -increasing;
- A number  $0 < a \leq \min\{F(i) : i \in \mathcal{V}\}$ .

Then, the matrix  $U$  defined as

$$U_{ij} = \begin{cases} F(i \overset{r}{\wedge} j) & \text{if } i, j \in \mathbb{T}_s[r] \\ F(i \overset{s}{\wedge} j) & \text{if } i, j \in \mathbb{T}_r[s] \\ a & \text{otherwise} \end{cases}$$

is called a **tree ultrametric matrix** with characteristic  $(\mathbb{T}, r, s, F, a)$ .

If  $r \neq s$  but  $a = F(r)$  we have  $F$  is  $r$ -increasing. Similarly, if  $r \neq s$  and  $a = F(s)$  then  $F$  is  $s$ -increasing. Also, when  $r = s$  we have  $F$  is  $r$ -increasing. In these cases we say that  $U$  is in **class 1** and its characteristic is denoted by  $(\mathbb{T}, r, F)$  (respectively  $(\mathbb{T}, s, F)$ ). When  $r \neq s$  and  $0 < a < \min\{F(i) : i \in \mathcal{V}\}$  we say that  $U$  is in **class 2**.

**Remark 3.1.** As we shall see classes 1 and 2 refer to the number of roots of  $U^{-1}$  (see [Theorem 3.4](#) (i.2) and [Theorem 3.5](#) (i.2)). Of course one can consider class  $p$ , as the set of ultrametric matrices with  $p$  roots. But then, according to [Theorem 3.7](#) and [Corollary 3.8](#), the set of roots is a complete graph, implying that for  $p \geq 3$  the underline graph of  $U^{-1}$  cannot be a tree.

Notice that the function  $F$  is obtained from the diagonal of  $U$  simply by  $F(i) = U_{ii}$ . This class of matrices is a special subclass of what Nabben in [19] called **tree structure**. See [Theorem 3.5](#) and [Corollary 3.6](#) in the cited paper, where a representation of a nonsingular matrix  $U$  of tree structure, is done in terms of Hadamard products of special matrices.

It is not hard to prove that every tree ultrametric matrix is an ultrametric matrix. We shall prove that every nonsingular ultrametric matrix  $U$ , that is the potential of a random walk on a tree, is a tree ultrametric matrix. Moreover,  $U$  has one or two roots. In the first case  $U$  is in class 1. If we denote its characteristic  $(\mathbb{T}, r, F)$ , then  $\mathcal{R}(U) = \{r\}$ , that is, the support of  $\mu_U$  is  $\{r\}$  and  $\mu_U = \bar{\mu}e_r = \frac{1}{F(r)}e_r$ , where  $e_r$  is the vector whose components are all zero, except the one associated with  $r$ , which is one. We also notice that in this case the row in  $U$  associated with  $r$  is constant and its value is  $F(r)$ , which is the minimum value of  $F$ . In the second case,  $U$  is in class 2 and  $\mathcal{R}(U) = \{r, s\}$ , where the characteristic of  $U$  is  $(\mathbb{T}, r, s, F, a)$ .

We shall use several times the following simple lemma.

**Lemma 3.3.** *Assume that  $\mathbb{T}$  is a tree and  $U$  is a class 1 tree ultrametric matrix with characteristic  $(\mathbb{T}, r, F)$ . If  $\mathbb{L} \subset \mathbb{T}$  is a subtree, then  $U|_{\mathbb{L}}$  is a class 1 tree ultrametric matrix with characteristic  $(\mathbb{L}, s, G)$  where  $s \in \mathbb{L}$  is the closest point to  $r$  and  $G = F|_{\mathbb{L}}$ .*

*If  $U, V$  are two class 1 tree ultrametric matrices with characteristics  $(\mathbb{T}, r, F)$  and  $(\mathbb{T}, r, G)$ , then  $U \odot V$  is a class 1 tree ultrametric matrix with characteristic  $(\mathbb{T}, r, FG)$ . Similarly, for any  $\alpha > 0$  the matrix  $U^{(\alpha)}$  is a class 1 tree ultrametric matrix with characteristic  $(\mathbb{T}, r, F^\alpha)$ .*

Every matrix  $U$  of class 2 is obtained from two matrices of class 1 and an extra number  $a$  in the following way. Assume that  $\mathbb{L}$  and  $\mathbb{M}$  are two disjoint trees. Assume that  $X$  and  $Y$  are two class 1 tree ultrametric matrices with characteristic  $(\mathbb{L}, r, G)$  and  $(\mathbb{M}, s, H)$ , respectively, and  $0 < a < \min\{G(r), H(s)\}$ . Consider the tree  $\mathbb{T}$  constructed by joining  $\mathbb{L}$  and  $\mathbb{M}$  through the edge  $(r, s)$ , then the matrix described by blocks as

$$U = \begin{pmatrix} X & a \\ a & Y \end{pmatrix}$$

is a class 2 tree ultrametric matrix with characteristic  $(\mathbb{T}, r, s, F, a)$ , where

$$F(i) = \begin{cases} G(i) & \text{if } i \in \mathbb{L} \\ H(i) & \text{if } i \in \mathbb{M} \end{cases}.$$

The class 1 tree ultrametric matrices are an extension of the class of **weighted tree ultrametric matrices** introduced in [4], where  $F$  is defined from the weight function by the relation  $F(i) = w(h_r(i))$ . In this way  $F(i)$  only depends on the height of  $i$ . We shall denote by  $(\mathbb{T}, r, w)$  the characteristic of a weighted tree ultrametric matrix. Notice that  $w : \{0, \dots, \mathbf{H}_r(\mathbb{T})\} \rightarrow \mathbb{R}^+$  is an increasing function. The next result is essentially proved in Theorem 2 in the cited paper (see also formulas (2.2) in [8]).

**Theorem 3.4.**

- (i) Assume that  $U$  is a class 1 tree ultrametric matrix with characteristic  $(\mathbb{T}, r, F)$  then
  - (i.1)  $U$  is nonsingular if and only if  $F$  is strictly  $r$ -increasing, that is if  $i \in \text{geod}_{\mathbb{T}}(j, r)$  and  $i \neq j$  then  $F(i) < F(j)$ ;
  - (i.2) If  $U$  is nonsingular then  $U$  is a potential with  $\mathbb{G}(U) = \mathbb{T}$ ,  $r$  is the unique root of  $U$  and

$$U_{ij}^{-1} = \begin{cases} \left. \begin{array}{l} \frac{-1}{U_{ii}-U_{jj}} & : i \in S_r(j) \\ \frac{-1}{U_{jj}-U_{ii}} & : j \in S_r(i) \\ \frac{1}{U_{ii}-U_{i-i}} + \sum_{k \in S_r(i)} \frac{1}{U_{kk}-U_{ii}} & : i = j \end{array} \right\} & \text{if } i \neq r; \\ \left. \begin{array}{l} \frac{-1}{U_{jj}-U_{rr}} & : j \in S_r(r) \\ \frac{1}{U_{rr}} + \sum_{k \in S_r(r)} \frac{1}{U_{kk}-U_{rr}} & : j = r \end{array} \right\} & \text{if } i = r. \end{cases} \quad (3.1)$$

- (ii) Assume  $\mathbb{T}$  is a tree and  $P$  is an irreducible symmetric substochastic matrix supported by  $\mathbb{T}$  and stochastic except at a unique node  $r \in \mathbb{T}$ , that is for all  $i \neq r$  the row sum  $\sum_j P_{ij} = 1$  and  $\sum_j P_{rj} < 1$ . Then  $U = (\mathbb{I} - P)^{-1}$  is a class 1 tree ultrametric matrix with characteristic  $(\mathbb{T}, r, F)$  where  $F(i) = U_{ii}$  for all  $i$ . The following is a formula for  $F$  in terms of  $P$

$$\begin{aligned} F(r) &= (1 - \sum_j P_{rj})^{-1} \\ F(j) &= F(r) + \sum_{t=0}^{p-1} (P_{i_t i_{t+1}})^{-1}, \end{aligned} \quad (3.2)$$

where  $\text{geod}_{\mathbb{T}}(j, r) = \{i_0 = r, \dots, i_p = j\}$ .

**Remark 3.2.** Let us give a probabilistic insight to Formula (3.1). So, consider  $j$  a successor of  $i$ . Take  $k \neq i$  a neighbor of  $j$ . The tree structure implies that any path starting at  $k$

must cross  $j$  until reaching the root  $r$ . Therefore,  $\mathbb{P}_k(\tau_j < \infty) = 1$  and we obtain  $U_{kj} = U_{jj}$ . Similarly, one has  $U_{ji} = U_{ii}$ . Then, the equation  $\sum_k U_{jk}U_{kj}^{-1} = 1$  implies that

$$U_{ii}U_{ij}^{-1} + U_{jj} \sum_{k \neq i} U_{kj}^{-1} = 1.$$

Since  $U^{-1}$  does not lose mass at  $j$ , we conclude  $\sum_{k \neq i} U_{kj}^{-1} + U_{ij}^{-1} = 0$ , proving that

$$U_{ij}^{-1} = \frac{1}{U_{ii} - U_{jj}}.$$

Now, we shall give a characterization of class 2 tree ultrametric matrices (see also Theorem 3.5 in [17] for the non-symmetric case).

**Theorem 3.5.**

- (i) Assume that  $U$  is a class 2 tree ultrametric matrix with characteristic  $(\mathbb{T}, r, s, F, a)$  or equivalently, after a suitable permutation of rows and columns if necessary, defined by blocks as

$$U = \begin{pmatrix} X & a \\ a & Y \end{pmatrix}, \tag{3.3}$$

where:

- $X$  is a class 1 matrix with characteristic  $(\mathbb{L}, r, G)$ ,  $\mathbb{L} = \mathbb{T}_s[r], G = F|_{\mathbb{T}_s[r]}$ ;
- $Y$  is a class 1 tree ultrametric matrix with characteristic  $(\mathbb{M}, s, H)$ ,  $\mathbb{M} = \mathbb{T}_r[s], H = F|_{\mathbb{T}_r[s]}$ ;
- $0 < a < \min\{G(r), H(s)\}$ .

Then,

- (i.1)  $U$  is nonsingular if and only if  $X$  and  $Y$  are nonsingular, which is equivalent to  $F|_{\mathbb{T}_s[r]}$  being strictly  $r$ -increasing and  $F|_{\mathbb{T}_r[s]}$  being strictly  $s$ -increasing.
- (i.2) If  $U$  is nonsingular, then  $U$  is a potential with  $\mathbb{G}(U) = \mathbb{T}$ . The set of roots of  $U$  is  $\mathcal{R}(U) = \{r, s\}$ . A formula for  $U^{-1}$  is the same as in (3.1) except for:

$$\begin{cases} U_{rr}^{-1} = \frac{U_{ss}}{U_{rr}U_{ss} - U_{rs}^2} + \sum_{j \in S_r(r); j \neq s} \frac{1}{U_{jj} - U_{rr}} \\ U_{ss}^{-1} = \frac{U_{rr}}{U_{rr}U_{ss} - U_{rs}^2} + \sum_{j \in S_s(s); j \neq r} \frac{1}{U_{jj} - U_{ss}} \\ U_{rs}^{-1} = \frac{-U_{rs}}{U_{rr}U_{ss} - U_{rs}^2}. \end{cases} \tag{3.4}$$

As a converse we have.

(ii) Consider a tree  $\mathbb{T}$  and a symmetric irreducible substochastic matrix  $P$  supported by  $\mathbb{T}$ . Assume that  $P$  is stochastic except at the nodes  $r \neq s \in \mathbb{T}$ , that is,

$$\forall i \neq r, s \quad \sum_j P_{ij} = 1, \quad \text{and} \quad \sum_j P_{rj} < 1, \quad \sum_j P_{sj} < 1.$$

If  $(r, s) \in \mathbb{T}$  then  $U = (\mathbb{I} - P)^{-1}$  is a tree ultrametric matrix with characteristic  $(\mathbb{T}, r, s, F, a)$  where  $F(i) = U_{ii}$  for all  $i$  and  $a = U_{rs} < \min\{F(i) : i \in \mathbb{T}\}$ . Hence,  $U$  is a class 2 tree ultrametric matrix.

The following is a formula for  $F$  and  $a$  in terms of  $P$ :

First compute  $\alpha = (1 - \sum_{j \neq s} P_{rj})^{-1}$ ,  $\beta = (1 - \sum_{j \neq r} P_{sj})^{-1}$  and then

$$\begin{aligned} F(r) &= \frac{\alpha}{1 - \alpha\beta(P_{rs})^2}, \quad F(s) = \frac{\beta}{1 - \alpha\beta(P_{rs})^2}, \quad a = \frac{\alpha\beta P_{rs}}{1 - \alpha\beta(P_{rs})^2}, \\ F(j) &= F(z) + \sum_{t=0}^{p-1} (P_{i_t i_{t+1}})^{-1}, \end{aligned} \tag{3.5}$$

$j \in \mathbb{T}_s[r]$  and  $z = s$  if  $j \in \mathbb{T}_r[s]$ .

**Proof.** (i) We shall use the inverse of a matrix by blocks. We assume that  $X$  is of order  $m$  and  $Y$  is of order  $n$ . We denote by  $\mathbb{1}_m, \mathbb{1}_n$  the vectors of ones of sizes  $m, n$  respectively. Also we denote by  $e_r, e_s$  the vectors of size  $m, n$  respectively with zero components except at  $r, s$  where they have a one. The basic properties to find  $U^{-1}$  are  $Xe_r = F(r)\mathbb{1}_m, Ye_s = F(s)\mathbb{1}_n$ . Hence, similarly to (3.3), we decompose  $U^{-1}$  as

$$U^{-1} = \begin{pmatrix} \Gamma & z \\ z' & \Lambda \end{pmatrix}. \tag{3.6}$$

We have  $\Gamma = (X - \frac{a^2}{F(s)}\mathbb{1}_m\mathbb{1}'_m)^{-1}$ ,  $z' = -aY^{-1}\mathbb{1}_n\mathbb{1}'_m\Gamma$ . We notice that

$$\tilde{X} = X - \frac{a^2}{F(s)}\mathbb{1}_m\mathbb{1}'_m$$

is a class 1 tree ultrametric matrix with characteristic  $(\mathbb{L}, r, G - \frac{a^2}{F(s)})$ .

Since  $G - \frac{a^2}{F(s)} > 0$ , the matrix  $\tilde{X}$  is nonsingular if and only if  $G - \frac{a^2}{F(s)}$  is strictly  $r$ -increasing, which is equivalent to  $G$  being strictly  $r$ -increasing. This fact and formula (3.1) give the formula for  $\Gamma$ . In particular, one has  $U_{rr}^{-1}$  as in (3.4). In a similar way, we obtain  $U_{ss}^{-1}$ .

On the other hand, to compute  $z$ , we notice that

$$\left( X - \frac{a^2}{F(s)}\mathbb{1}_m\mathbb{1}'_m \right) e_r = \frac{F(r)F(s) - a^2}{F(s)} \mathbb{1}_m.$$

This fact yields

$$z' = \frac{-a}{F(r)F(s) - a^2} e_s e'_r$$

and we obtain  $U_{rs}^{-1} = \frac{-a}{F(r)F(s) - a^2}$  from where (3.4) holds.

According to what we have proved and Theorem 3.4,  $\mathbb{G}(U)$  is the tree obtained from the two trees  $\mathbb{L}$  and  $\mathbb{M}$  that are connected by adding the edge  $(r, s)$ . Finally, we obtain that  $\sum_j U_{ij}^{-1} = 0$  for all  $i \neq r, s$  and

$$\sum_j U_{rj}^{-1} = \frac{U_{rr} - U_{rs}}{U_{rr}U_{ss} - U_{rs}^2} > 0, \quad \sum_j U_{sj}^{-1} = \frac{U_{ss} - U_{rs}}{U_{rr}U_{ss} - U_{rs}^2} > 0,$$

proving that  $\mathcal{R}(U) = \{r, s\}$ .

(ii) The hypotheses made on  $P$  ensure that  $\mathbb{I} - P$  is nonsingular. Again we decompose this matrix by blocks as

$$\mathbb{I} - P = \begin{pmatrix} \mathbb{I}_m - Q & -P_{rs}e_r e'_s \\ -P_{rs}e_s e'_r & \mathbb{I}_n - R \end{pmatrix}.$$

$Q$  and  $R$  are irreducible substochastic matrices supported by  $\mathbb{L}$  and  $\mathbb{M}$  respectively. Moreover  $Q$  is stochastic except at  $r$  and  $R$  is stochastic except at  $s$ . Thus, Theorem 3.4 shows that  $\mathbb{I}_m - Q$  and  $\mathbb{I}_n - R$  are nonsingular and their inverses are class 1 tree ultrametric matrices. The first block of  $U = (\mathbb{I} - P)^{-1}$  is

$$X = [\mathbb{I}_m - Q - P_{rs}^2 e_r e'_s (\mathbb{I}_n - R)^{-1} e_s e'_r]^{-1}.$$

Notice that

$$(\mathbb{I}_n - R)\mathbf{1}_n = \left(1 - \sum_{j \neq r} P_{sj}\right) e_s = \frac{1}{\beta} e_s.$$

Therefore we obtain

$$X = [\mathbb{I}_m - (Q + \beta P_{rs}^2 e_r e'_s)]^{-1}$$

The matrix  $Q + \beta P_{rs}^2 e_r e'_s$  is nonnegative and stochastic at every  $i \neq r$ . The row sum at  $r$  is

$$\sum_{j \neq s} P_{rj} + \beta P_{rs}^2 = \sum_{j \neq s} P_{rj} + P_{rs} \frac{P_{rs}}{1 - \sum_{j \neq s} P_{rj}} \leq \sum_{j \neq s} P_{rj} + P_{rs} < 1.$$

The conclusion is that  $Q + \beta P_{rs}^2 e_r e'_s$  is stochastic except at  $r$ . Since this matrix is supported by the tree  $\mathbb{L}$  we obtain that  $X$  is a class 1 tree ultrametric matrix with characteristic  $(\mathbb{L}, r, G)$ . A formula for  $G$  is given by (3.2)



$$G(r) = \left(1 - \sum_{j \neq s} P_{rj} - \beta P_{rs}^2\right)^{-1} = \frac{\alpha}{1 - \alpha\beta P_{rs}^2},$$

$$G(j) = G(r) + \sum_{t=0}^{p-1} (P_{i_t i_{t+1}})^{-1},$$

where  $geod_{\mathbb{T}}(j, r) = geod_{\mathbb{L}}(j, r) = \{i_0 = r, \dots, i_p = j\}$  if  $j \in \mathbb{T}_s[r] = \mathbb{L}$ .

In the same way,  $Y$  is a class 1 tree ultrametric matrix with characteristic  $(\mathbb{M}, s, H)$  and  $H$  is computed similarly to  $G$ . In particular  $H(s) = \frac{\beta}{1 - \alpha\beta P_{rs}^2}$ .

Finally,

$$U = \begin{pmatrix} X & A \\ A' & Y \end{pmatrix},$$

with  $A = P_{rs}(\mathbb{I}_m - Q)^{-1}e_r e'_s Y$ . Since  $(\mathbb{I}_m - Q)\mathbb{1}_m = \frac{1}{\alpha}e_r$  and  $e'_s Y = H(s)\mathbb{1}'_n$  we get  $A = a\mathbb{1}_m\mathbb{1}_n$  with

$$a = H(s)P_{rs}\alpha = \frac{\alpha\beta P_{rs}}{1 - \alpha\beta P_{rs}^2}.$$

On the other hand, from  $\alpha P_{rs} < 1$  and  $\beta P_{rs} < 1$ , we conclude that  $a < \min\{G(r), H(s)\}$  and the result is proved.  $\square$

As a corollary of [Theorem 2.1](#) we have the following result.

**Corollary 3.6.** *If  $U$  is a class 2 ultrametric matrix with roots  $r, s$ , then there exist two class 1 ultrametric matrices  $V, Z$ , with roots  $r$  and  $s$  respectively, such that*

$$U = V \odot Z.$$

See [Appendix A](#) where we provide an explicit decomposition of  $U$  as the product of two class 1 ultrametric matrices.

To finish the characterization of ultrametric matrices supported by a tree, we need the following theorem (see [\[4\]](#), Theorem 2 and also [\[5\]](#) for some generalizations). This result says that every ultrametric matrix is the restriction of some weighted tree matrix. This representation gives information on the graph of the given ultrametric matrix.

**Theorem 3.7.** *Given any ultrametric matrix  $V$  on a set  $I$ , there exists (a minimal) extension  $U$ , which is a weighted tree ultrametric matrix with characteristic  $(\mathbb{T}, r, w)$ , such that  $I \subset \mathbb{T}$  and  $V = U|_I$ .  $V$  is nonsingular if and only if  $w$  is strictly increasing and positive. In this case  $V$  is a potential matrix and the roots of  $V$  are characterized as*

$$i \in \mathcal{R}(V) \iff geod_{\mathbb{T}}(i, r) \cap I = \{i\}.$$

Also, if  $i \neq j \in \mathcal{R}(V)$  then  $V_{ij}^{-1} < 0$ , that is, the roots of  $V$  are all connected in  $\mathbb{G}(V)$ . More generally, for  $i \neq j \in I$  we have  $V_{ij}^{-1} < 0$  if and only if  $geod_{\mathbb{T}}(i, j) \cap I = \{i, j\}$ .

**Corollary 3.8.** *Assume  $U$  is a nonsingular ultrametric matrix supported on a tree  $\mathbb{T}$ . Then, the set of roots of  $U$  is a singleton or it consists of two points  $r, s$  which are neighbors in  $\mathbb{T}$ . In the first case  $U$  is in class 1 and in the second case  $U$  is in class 2.*

**Proof.** According to Theorem 3.7, the set of roots of  $U$  forms a complete subgraph of  $\mathbb{T}$ . Then either this set is a singleton or it consists of two neighboring nodes.  $\square$

**4. Proof of Theorem 2.1**

(i) Assume that  $W^{-1} = M$  is an  $M$ -matrix supported on the tree  $\mathbb{T}$ . First, let us find a diagonal matrix  $F$  such that  $FW$  is a potential. For that purpose it is enough to take any nonnegative vector  $x \in \mathbb{R}^n$ , which is not 0, and consider  $F_{ii} = \frac{1}{(Wx)_i}$  (this is well defined because  $Wx > 0$ ). Then  $FWx = \mathbb{1}$ , which means that  $(FW)^{-1}$  is an  $M$ -matrix and  $(FW)^{-1}\mathbb{1} = x \geq 0$ , that is  $(FW)^{-1}$  is a row diagonally dominant matrix. In summary,  $FW$  is a potential. Notice also that  $\mathbb{G}(FW) = \mathbb{G}(W)$ , because a diagonal matrix does not change this graph. On the other hand if  $W$  is a potential we can take  $F = \mathbb{I}$ , which corresponds to  $x = \mu_W$ , the equilibrium potential of  $W$ .

We now show how to construct a positive diagonal matrix  $E$  such that  $WE$  is a symmetric inverse  $M$ -matrix supported on the same tree  $\mathbb{T}$ . Further, if  $W$  is a potential we show that  $WE$  is again a potential. This will finish the proof of (i).

For the moment fix a vertex  $r \in \mathbb{T}$ . We define the following diagonal matrix  $L$ :  $L_{rr} = 1$  and for  $k \in \mathbb{T}$

$$L_{kk} = \prod_{\ell=0}^{p-1} \frac{M_{i_\ell, i_{\ell+1}}}{M_{i_{\ell+1}, i_\ell}} > 0,$$

where the geodesic from  $r$  to  $k$  is  $r = i_0, \dots, i_p = k$ .

Now, we take  $i \neq k$  neighbors in  $\mathbb{T}$ . We assume without loss of generality that  $geod_{\mathbb{T}}(r, k)$  passes through  $i$ , that is  $geod_{\mathbb{T}}(r, k) = \{i_0 = r, \dots, i_{p-1} = i, i_p = k\}$ . Hence,

$$L_{kk} = L_{ii} \frac{M_{ik}}{M_{ki}},$$

or equivalently  $L_{ii}M_{ik} = L_{kk}M_{ki}$ . Now, the fact that  $M$  is supported on  $\mathbb{T}$  shows that  $LM$  is a symmetric  $M$ -matrix, which is supported on  $\mathbb{T}$ . Thus, its inverse  $WL^{-1}$  is a symmetric inverse  $M$ -matrix. If  $M$  is row diagonally dominant, this means  $W$  is a potential, then  $M\mathbb{1} \geq 0$ , but then again  $LM\mathbb{1} \geq 0$ , which shows that  $WL^{-1}$  is a symmetric potential.

(ii) Consider the matrix  $U = \text{diag}(1./W_{\bullet r})W\text{diag}(1./W_{r\bullet})$ , which is the matrix given by

$$U_{ij} = \frac{W_{ij}}{W_{ir}W_{rj}}.$$

We claim this is a symmetric potential. Indeed, as we have proved in (i) there is a diagonal matrix  $G$  such that  $WG$  is symmetric. This implies that, for all  $s, t$

$$W_{st}G_{tt} = W_{ts}G_{ss}.$$

In particular,  $W_{sr}G_{rr} = W_{rs}G_{ss}$ , or equivalently  $G_{ss} = G_{rr} \frac{W_{sr}}{W_{rs}}$  (the value of  $G_{rr}$  is free). Now, from  $W_{ij}G_{jj} = W_{ji}G_{ii}$ , we obtain

$$W_{ij}G_{rr} \frac{W_{jr}}{W_{rj}} = W_{ji}G_{rr} \frac{W_{ir}}{W_{ri}},$$

showing that  $U$  is symmetric. The fact that  $U^{-1}$  is an  $M$ -matrix is straightforward. So, we need to show that  $U^{-1}$  is a row diagonally dominant matrix or equivalently the unique solution to  $U\mu = \mathbb{1}$  is a nonnegative vector  $\mu$ . This follows from the fact  $Ue_r = \frac{1}{W_{rr}}\mathbb{1}$ , where  $e_r$  is the vector whose components are all zeros, except the one at position  $r$ , which is 1. So,  $U$  is a symmetric potential and it has a unique root at  $r$ .

On the other hand,  $\mathbb{G}(U) = \mathbb{G}(W) = \mathbb{T}$  is a tree, that is,  $U$  is proportional to the potential of a symmetric Markov chain on the tree  $\mathbb{T}$  that loses mass only at the point  $r$ . According to [Theorem 3.4 \(ii\)](#)  $U$  is a class 1 tree ultrametric matrix.

(iii) We assume that  $W$  is a symmetric potential. In particular,  $W^{-1} = k(\mathbb{I} - P)$ , where  $k > 0$  is a constant,  $P$  is a substochastic matrix supported by  $\mathbb{T}$ . Without loss of generality we assume that  $k = 1$ . We denote by  $X = (X_m : m \in \mathbb{N})$  the Markov chain with transition kernel  $P$ . We also denote by  $\tau = \min\{m \geq 0 : X_m \notin I\}$  the absorption time for this chain, which is finite almost surely because  $X$  is transient. Also, we denote by  $\tau_k = \min\{m \geq 0 : X_m = k\}$ , the hitting time of  $k \in \mathbb{T}$ .

We prove the result by induction on  $n$ , the order of  $W$ . We notice that for  $n \leq 3$  the tree  $\mathbb{T}$  is a path and the result is obtained from [Theorem 2.1](#) in [\[9\]](#). So in what follows we assume the result is true for potentials of order smaller or equal to  $n - 1$  and  $n \geq 4$ .

We shall distinguish two main cases: (I) assume there is a leaf  $t \notin \mathcal{R}(W)$ , and (II)  $\mathcal{L}(\mathbb{T}) \subset \mathcal{R}(W)$ .

(I) Consider  $\mathbb{L} = \mathbb{T} \setminus \{t\}$ , which is a tree because  $t$  is a leaf. The matrix  $Z = W|_{\mathbb{L}}$  satisfies the induction hypothesis, because it is the potential of the induced Markov chain on  $\mathbb{L}$ , which has a symmetric transition kernel supported on the tree  $\mathbb{L}$ . This induced Markov chain consists simply in recording the visits to  $\mathbb{L}$  for the original chain (see [Section 2.2](#), [Proposition 2.22](#) in [\[10\]](#)). Hence, for every  $\ell \in \text{ext}(\mathcal{R}(Z))$  there exists a class 1 tree ultrametric matrix  $V_\ell$ , of order  $n - 1$ , supported by  $\mathbb{L}$  whose unique root is  $\ell$  and such that

$$Z = \bigoplus_{\ell \in \text{ext}(\mathcal{R}(Z))} V_\ell.$$

We extend each one of these matrices to dimension  $n$ . We call these extensions  $(U_\ell : \ell \in \text{ext}(\mathcal{R}(Z)))$ , which are obtained by adding a row and a column associated with  $t$  as follows

$$(U_\ell)_{ti} = (U_\ell)_{it} = \begin{cases} (V_\ell)_{si} & \text{if } i \neq t \\ \theta_\ell & \text{if } i = t, \end{cases}$$

where  $s$  is the unique neighbor of  $t$  in  $\mathbb{T}$ . For the moment we demand that

$$\theta_\ell > (V_\ell)_{ss} = \max\{(V_\ell)_{si} : i \in \mathbb{L}\}.$$

We notice that  $s \in \text{geod}_{\mathbb{T}}(t, k)$  for any  $k \neq t$ . From this observation, it is straightforward to show that if  $V_\ell$  has characteristic  $(\mathbb{L}, \ell, F_\ell)$  then  $U_\ell$  has characteristic  $(\mathbb{T}, \ell, G_\ell)$ , where  $G_\ell$  is the extension of  $F_\ell$  to  $\mathbb{T}$  given by  $G_\ell(t) = \theta_\ell$ . Since  $G_\ell$  is a strictly  $\ell$ -increasing function, we deduce that  $U_\ell$  is proportional to a symmetric potential of a Markov chain in  $\mathbb{T}$  with a unique root  $\ell$ . Hence,  $U_\ell$  is a class 1 tree ultrametric matrix. Let us prove that for some selection of  $\theta_\ell : \ell \in \text{ext}(\mathcal{R}(Z))$ , we have

$$W = \bigodot_{\ell \in \text{ext}(\mathcal{R}(Z))} U_\ell.$$

We only have to prove that equality holds at entries  $(t, i)$ . On the one hand, if  $i \neq t$ , we have

$$W_{ti} = \mathbb{P}_t(\tau_s < \infty)W_{si} = W_{si} = \prod_{\ell \in \text{ext}(\mathcal{R}(Z))} (V_\ell)_{si} = \prod_{\ell \in \text{ext}(\mathcal{R}(Z))} (U_\ell)_{si} = \prod_{\ell \in \text{ext}(\mathcal{R}(Z))} (U_\ell)_{ti}.$$

In this equality we have used the fact that  $t$  is not a root of  $W$ , which implies that the chain associated with  $W$  and starting at  $t$  visits  $s$  with probability 1. The same argument shows that  $(U_\ell)_{si} = (U_\ell)_{ti}$  for all  $i \neq t$ .

On the other hand, notice that  $W_{st} = \mathbb{P}_s(\tau_t < \infty)W_{tt} < W_{tt}$ , because there is a path starting from  $s$ , that does not pass through  $t$  and that reaches some root of  $W$ . So,  $\mathbb{P}_s(\tau_t < \infty) < 1$ . The symmetry of  $W$  implies that  $W_{st} = W_{ts} = W_{ss}$ . Hence,  $W_{tt} > W_{ss} = \prod_{\ell \in \text{ext}(\mathcal{R}(Z))} (V_\ell)_{ss}$ , so it is possible to choose  $\theta_\ell : \ell \in \text{ext}(\mathcal{R}(Z))$  to fit the value

$$W_{tt} = \prod_{\ell \in \text{ext}(\mathcal{R}(Z))} \theta_\ell.$$

The result is proven in case (I) by noticing that  $\text{ext}(\mathcal{R}(Z)) = \text{ext}(\mathcal{R}(W))$ , because  $\mathcal{R}(Z) = \mathcal{R}(W)$ .

(II) In this case all leaves of  $\mathbb{T}$  are roots for  $W$  and  $\text{ext}(\mathcal{R}(W)) = \mathcal{L}(\mathbb{T})$ . For the moment, we fix a node  $a \in \mathbb{T}$ , which is not a leaf. Take any leaf  $t$ , which is at a maximal distance from  $a$ , and consider  $s$  its unique neighbor. Then, the set

$$\mathcal{A} = \{\ell \in \mathcal{L}(\mathbb{T}) : d_{\mathbb{T}}(s, \ell) = 1\} = \{t_1, \dots, t_p\}$$

contains  $t$  and has cardinal  $p \geq 1$ .

We consider the subtree  $\mathbb{L} = \mathbb{T} \setminus \mathcal{A}$ , for which  $s$  must be a leaf, otherwise it contradicts the maximality of  $t$ . It is clear that  $\mathcal{L}(\mathbb{L}) = \{s\} \cup \mathcal{L}(\mathbb{T}) \setminus \mathcal{A}$  and  $\mathcal{L}(\mathbb{T}) = \mathcal{A} \cup \mathcal{L}(\mathbb{L}) \setminus \{s\}$ .

We take  $Z = W|_{\mathbb{L}}$ , which corresponds to the potential of the induced Markov chain on  $\mathbb{L}$ . This induced Markov chain is denoted by  $Y = (Y_m : m \in \mathbb{N})$ . Its transition probability kernel  $Q$  is for  $i, j \in \mathbb{L}$

$$\mathbb{P}_i(Y_1 = j) = Q_{ij} = \mathbb{P}_i(X \text{ returns to } \mathbb{L}, \text{ before absorption, at } j).$$

Notice that  $Q_{ij} = P_{ij}$  for all  $(i, j) \neq (s, s)$ , which proves that  $Q$  is supported on  $\mathbb{L}$ . The nodes where this induced chain loses mass are those where the original chain loses mass in  $\mathbb{L}$  plus the node  $s$ . The latter case holds true because, for the original chain, the probability that the first transition starting from  $s$  reaches  $t$  is  $P_{st} > 0$ , which gives the following lower bound for the row sum of  $Z^{-1}$  at row  $s$  (notice that  $t \notin \mathbb{L}$ )

$$\begin{aligned} \sum_{k \in \mathbb{L}} Z_{sk}^{-1} &= \mathbb{P}_s(Y \text{ is absorbed in one step}) \\ &\geq P_{st} \mathbb{P}_t(X \text{ is absorbed in one step}) = P_{st} \sum_{k \in \mathbb{T}} W_{tk}^{-1} > 0. \end{aligned}$$

Hence, the roots of  $Z$  are the roots of  $W$  in  $\mathbb{L}$  plus  $s$  which implies that  $\text{ext}(\mathcal{R}(Z)) = \mathcal{L}(\mathbb{L})$ . Then, the induction hypothesis implies that

$$Z = \bigoplus_{\ell \in \mathcal{L}(\mathbb{L})} V_{\ell},$$

for some collection of class 1 tree ultrametric matrices  $V_{\ell} : \ell \in \mathcal{L}(\mathbb{L})$ . Each  $V_{\ell}$  has a unique root at  $\ell$  and  $\mathbb{G}(V_{\ell}) = \mathbb{L}$ . For  $\ell \in \mathcal{L}(\mathbb{L})$ , such that  $\ell \neq s$ , let  $U_{\ell}$  be the following extension of  $V_{\ell}$ :  $U_{\ell}|_{\mathbb{L}} = V_{\ell}$  and

$$(U_{\ell})_{ij} = (U_{\ell})_{ji} = \begin{cases} (V_{\ell})_{sj} & \text{if } i \in \mathcal{A}, j \in \mathbb{L} \\ (V_{\ell})_{ss} & \text{if } i \in \mathcal{A}, j \in \mathcal{A} \setminus \{i\} \\ \theta_{\ell i} & \text{if } i = j \in \mathcal{A}, \end{cases}$$

with the restriction that  $\theta_{\ell i} > (V_{\ell})_{ss}$  for all  $i \in \mathcal{A}$ . If the characteristic of  $V_{\ell}$  is  $(\mathbb{L}, \ell, F_{\ell})$ , then the characteristic of  $U_{\ell}$  is  $(\mathbb{T}, \ell, G_{\ell})$  where  $G_{\ell}$  is the extension of  $F_{\ell}$  given by  $G_{\ell}(i) = \theta_{\ell i}$  for  $i \in \mathcal{A}$ . It is straightforward to show that  $G_{\ell}$  is a strictly  $\ell$ -increasing function on  $\mathbb{T}$ .

The extension for  $V_s$  is more complicated. This matrix will generate  $p$  new matrices that we denote by  $U_{t_k} : k = 1, \dots, p$ . All of them agree on  $\mathbb{L}$  and are given by the  $1/p$  Hadamard power of  $V_s$ , that is,  $(U_{t_k})|_{\mathbb{L}} = V_s^{(1/p)}$ . In order to define these extensions we consider  $\alpha_{t_k} = \mathbb{P}_{t_k}(\tau_s < \infty) < 1$ , for  $k = 1, \dots, p$ . Then,  $U_{t_k}$  is defined as

$$(U_{t_k})_{ij} = (U_{t_k})_{ji} = \begin{cases} (V_s)^{1/p}_{ss} & \text{if } i \in \mathcal{A} \setminus \{t_k\}, j \in \mathbb{T} \setminus \{i\} \\ \alpha_{t_k} (V_s)^{1/p}_{ss} & \text{if } i = t_k, j \in \mathbb{T} \\ \theta_{t_k i} & \text{if } i = j \in \mathcal{A} \setminus \{t_k\}, \end{cases}$$

with the restriction that  $\theta_{t_k t_l} > (V_s)^{1/p}_{ss}$ , for  $l = 1, \dots, p$  and  $l \neq k$ .

Each  $U_{t_k}$  is a class 1 tree ultrametric matrix. Indeed, if the characteristic of  $V_s$  is  $(\mathbb{L}, s, F_s)$  then  $U_{t_k}$  has characteristic  $(\mathbb{T}, t_k, G_{t_k})$  where  $G_{t_k}$  is given by:  $G_{t_k}|_{\mathbb{L}} = F_s^{1/p}$ ;  $G_{t_k}(t_k) = \alpha_{t_k} F_s(s)^{1/p}$  and  $G_{t_k}(t_l) = \theta_{t_k t_l} > G_{t_k}(s) = F_s^{1/p}(s) > G_{t_k}(t_k)$ , for  $t_l \neq t_k$ . The function  $G_{t_k}$  is strictly  $t_k$ -increasing in  $\mathbb{T}$ .

Take now  $\Gamma = \bigodot_{\ell \in \mathcal{L}(\mathbb{T})} U_\ell$ . We shall prove that  $W = \Gamma$  for some choice of

$$\{\theta_{t_k t_l} : t_k, t_l \in \mathcal{A}, t_k \neq t_l\} \cup \{\theta_{\ell t_k} : \ell \in \mathcal{L}(\mathbb{L}) \setminus \{s\}, t_k \in \mathcal{A}\}.$$

For that purpose, consider first  $i, j \in \mathbb{L}$ . Then,

$$\Gamma_{ij} = \prod_{\ell \in \mathcal{L}(\mathbb{T})} (U_\ell)_{ij} = [(V_s)_{ij}^{1/p}]^p \prod_{\ell \in \mathcal{L}(\mathbb{L}), \ell \neq s} (V_\ell)_{ij} = \prod_{\ell \in \mathcal{L}(\mathbb{L})} (V_\ell)_{ij} = Z_{ij} = W_{ij}.$$

Now, we consider  $i = t_k \in \mathcal{A}, j \in \mathbb{L}$

$$\Gamma_{t_k j} = \alpha_{t_k} (V_s)_{ss}^{1/p} \prod_{t_l \in \mathcal{A}, l \neq k} (V_s)_{ss}^{1/p} \prod_{\ell \in \mathcal{L}(\mathbb{L}) \setminus \{s\}} (V_\ell)_{sj} = \alpha_{t_k} \prod_{\ell \in \mathcal{L}(\mathbb{L})} (V_\ell)_{sj}.$$

The last equality follows from the fact that  $(V_s)_{sj} = (V_s)_{ss}$ . Hence, we get

$$\Gamma_{t_k j} = \alpha_{t_k} Z_{sj} = \alpha_{t_k} W_{sj} = \mathbb{P}_{t_k}(\tau_s < \infty) W_{sj} = W_{t_k j}.$$

When  $i = t_k, j = t_l \in \mathcal{A}, k \neq l$ , we obtain

$$\begin{aligned} \Gamma_{t_k t_l} &= \alpha_{t_k} \alpha_{t_l} (V_s)_{ss} \prod_{\ell \in \mathcal{L}(\mathbb{L}) \setminus \{s\}} (V_\ell)_{ss} = \alpha_{t_k} \alpha_{t_l} \prod_{\ell \in \mathcal{L}(\mathbb{L})} (V_\ell)_{ss} = \alpha_{t_k} \alpha_{t_l} Z_{ss} \\ &= \alpha_{t_k} \alpha_{t_l} W_{ss} = \mathbb{P}_{t_k}(\tau_s < \infty) \mathbb{P}_{t_l}(\tau_s < \infty) W_{ss} = \mathbb{P}_{t_k}(\tau_s < \infty) W_{t_l s} \\ &= \mathbb{P}_{t_k}(\tau_s < \infty) W_{st_l} = W_{t_k t_l}. \end{aligned}$$

We are finally left with the case  $i = j = t_k$

$$\Gamma_{t_k t_k} = \alpha_{t_k} [(V_s)_{ss}]^{1/p} \prod_{t_l \in \mathcal{A} \setminus t_k} \theta_{t_l t_k} \prod_{\ell \in \mathcal{L}(\mathbb{L}) \setminus \{s\}} \theta_{\ell t_k}$$

We notice that given the restrictions satisfied by the family of parameters  $\theta$ , then

$$\Gamma_{t_k t_k} > \alpha_{t_k} \prod_{\ell \in \mathcal{L}(\mathbb{L})} (V_\ell)_{ss} = \alpha_{t_k} W_{ss} = W_{t_k s}.$$

On the other hand  $W_{st_k} = \mathbb{P}_s(\tau_{t_k} < \infty) W_{t_k t_k} < W_{t_k t_k}$ . This last inequality follows from the fact that  $s$  is connected to  $\ell \neq t_k$ , a root of  $W$ , with a path that does not pass throughout  $t_k$ . Therefore,  $\mathbb{P}_s(\tau_{t_k} = \infty) > \mathbb{P}_s(\tau_\ell < \tau_{t_k}) \mathbb{P}_\ell(\tau_{t_k} = \infty) > 0$ . Thus, there is a possible choice of  $\theta_{t_l t_k} : l \neq k$  and  $\theta_{\ell t_k} : \ell \in \mathcal{L}(\mathbb{L}) \setminus \{s\}$  such that  $\Gamma_{t_k t_k} = W_{t_k t_k}$  and the result is shown.  $\square$

**5. Proof of Theorem 2.2**

The idea of the proof is first to show (i) by induction on  $n$ , the cardinality of  $\mathbb{T}$ . Then, use again induction for (ii) and (iii) and some computations done while proving (i).

Notice that the result is obvious when  $n \leq 2$ . Also, the case where the cardinal of  $\mathcal{A}$  is one is direct because in this case  $W$  is ultrametric. So, in what follows we assume that  $n \geq 3$  and  $|\mathcal{A}| \geq 2$ .

(i) Since every  $U_\ell$  is an inverse  $M$ -matrix, then they are positive definite and therefore  $W$  is also a positive definite matrix and a fortiori nonsingular. Moreover, every principal submatrix of  $W$ , associated with an index set  $J \subset \mathbb{T}$ , is nonsingular and it is the Hadamard product of class 1 tree ultrametric matrices, which are the corresponding blocks of the matrices  $(U_\ell : \ell \in \mathcal{A})$ . Maybe the index set  $\mathcal{A}$  is not a subset of  $J$ , nevertheless we can reparametrize these blocks with a subset of  $J$  (see Lemma 3.3). We shall use this fact to compute the inverse of  $W$  by blocks.

Take any leaf  $t \in \mathbb{T}$  and consider the subtree  $\mathbb{L} = \mathbb{T} \setminus \{t\}$ . We denote by  $s \in \mathbb{T}, s \neq t$ , the unique neighbor of  $t$  in  $\mathbb{T}$ . After a permutation, if necessary, we can assume that  $W$  can be decomposed in blocks like

$$W = \begin{pmatrix} a & w' \\ w & Z \end{pmatrix},$$

where the first row of  $W$  is the one associated with  $t$ . For any  $i \neq t$  we have  $(U_\ell)_{ti} = \mathbb{P}_t(\tau_s^\ell < \infty)(U_\ell)_{si}$ . Here  $\tau_s^\ell$  is the hitting time of  $s$  for the Markov chain associated with  $U_\ell$ . In particular we have

$$\mathbb{P}_t(\tau_s^\ell < \infty) = \frac{(U_\ell)_{ts}}{(U_\ell)_{ss}},$$

and we conclude that

$$W_{ti} = w_i = \alpha Z_{si} = \alpha W_{si},$$

where  $\alpha = \frac{W_{ts}}{W_{ss}} = \prod_{\ell \in \mathcal{A}} \mathbb{P}_t(\tau_s^\ell < \infty) \leq 1$ .

The inverse by blocks of  $W$  is

$$W^{-1} = \begin{pmatrix} \theta & -\alpha\theta e'_s \\ -\alpha\theta e_s & Z^{-1} + \alpha^2\theta e_s e'_s \end{pmatrix}, \tag{5.1}$$

where  $\theta = \frac{1}{a - \alpha^2 Z_{ss}} = \frac{W_{ss}}{W_{tt}W_{ss} - W_{st}^2}$ , which we shall prove is positive and the first part of the result will follow, that is  $W^{-1}$  is an  $M$ -matrix. Notice that by induction the incidence graph of  $W^{-1}$  is  $\mathbb{T}$ .

That  $\theta$  is positive follows from the fact that the  $2 \times 2$  determinant

$$W_{tt}W_{ss} - W_{st}^2 = \left| \begin{pmatrix} W_{tt} & W_{st} \\ W_{st} & W_{ss} \end{pmatrix} \right|$$

is positive because  $W$  is positive definite. This shows part (i).

In what follows, that is in the proof of (ii), (iii), we need to study when  $\alpha = 1$  or  $\alpha < 1$ . For this purpose, we consider to different cases according to the fact that  $t$  belongs or not to  $\mathcal{A}$ , but still  $t$  is a leaf of  $\mathbb{T}$ .

Case  $t \notin \mathcal{A}$ . In this situation we have that  $\mathbb{P}_t(\tau_s^\ell < \infty) = 1$  for all  $\ell \in \mathcal{A}$ , that is  $\alpha = 1$ , because  $t$  is not the root of  $U_\ell$ . For the same reason we have  $(U_\ell)_{tt} > (U_\ell)_{st} = (U_\ell)_{ss}$  and therefore

$$a = W_{tt} = \prod_{\ell \in \mathcal{A}} (U_\ell)_{tt} > \prod_{\ell \in \mathcal{A}} (U_\ell)_{ss} = Z_{ss}.$$

Thus,  $a > \alpha^2 Z_{ss} = Z_{ss}$  and  $W^{-1}$  is an  $M$ -matrix, whose row sums are the same as the ones for  $Z^{-1}$ , on the common rows, and the row sum associated with  $t$  is 0.

Case  $t \in \mathcal{A}$ . Here,  $\mathbb{P}_t(\tau_s^\ell < \infty) = 1$  for all  $\ell \in \mathcal{A} \setminus \{t\}$  and  $\alpha = \mathbb{P}_t(\tau_s^t < \infty) < 1$ . As before

$$\begin{aligned} a = W_{tt} &= (U_t)_{tt} \prod_{\ell \in \mathcal{A} \setminus \{t\}} (U_\ell)_{tt} = (U_t)_{ts} \prod_{\ell \in \mathcal{A} \setminus \{t\}} (U_\ell)_{tt} \\ &= \alpha (U_t)_{ss} \prod_{\ell \in \mathcal{A} \setminus \{t\}} (U_\ell)_{tt} > \alpha (U_t)_{ss} \prod_{\ell \in \mathcal{A} \setminus \{t\}} (U_\ell)_{ss} = \alpha Z_{ss} > \alpha^2 Z_{ss}. \end{aligned}$$

The row sum for  $W^{-1}$  associated with  $t$  is positive, and the row sums of  $W^{-1}$  are the same as the ones corresponding to  $Z^{-1}$ , except at the row associated with  $s$ , which can have any sign.

Recall that we can express  $\theta, \alpha$  in terms of  $W$  as

$$\alpha = \frac{W_{ts}}{W_{ss}}, \theta = \frac{W_{ss}}{W_{tt}W_{ss} - W_{ts}^2}.$$

Now, we are in a position to continue with the proof of parts (ii) and (iii).

(ii) In case  $\mathbb{T}(\mathcal{A}) = \mathbb{T}$  the result is already proven, because in this situation there is nothing to prove for  $t \notin \mathbb{T}(\mathcal{A})$  and if  $t \in \text{ext}(\mathcal{A})$  then  $t$  is a leaf of  $\mathbb{T}$ , hence the row sum of  $W^{-1}$  at the row associated with  $t$  is positive. So, in this case (ii) holds.

Now, we consider the situation where  $\mathbb{T}(\mathcal{A})$  is a proper subtree of  $\mathbb{T}$ . We show that the row sums of  $(W|_{\mathbb{T}(\mathcal{A})})^{-1}$  and  $W^{-1}$  at rows associated with nodes in  $\mathbb{T}(\mathcal{A})$  are the same and the row sums of  $W^{-1}$  at the other nodes are 0. Indeed, consider  $\mathbb{L}_0 = \mathbb{T}(\mathcal{A})$  and take any node  $u \in \mathbb{T}$  such that  $d_{\mathbb{T}}(u, \mathbb{L}_0) = 1$ . Then,  $u$  is a leaf of the tree  $\mathbb{L}_1 = \mathbb{L}_0 \cup \{u\}$  and  $u \notin \mathcal{A}$ . Then, the row sums of  $(W|_{\mathbb{L}_0})^{-1}$  and  $(W|_{\mathbb{L}_1})^{-1}$  are the same at nodes in  $\mathbb{L}_0$  and the row sum of  $(W|_{\mathbb{L}_1})^{-1}$  at the row associated with  $u$  is 0. We continue adding nodes in this way and the claim is shown.

In particular, if  $t \notin \mathbb{T}(\mathcal{A})$  we conclude that the corresponding row sum of  $W^{-1}$  is 0. On the other hand if  $t \in \text{ext}(\mathcal{A})$ , then  $t$  is a leaf for  $\mathbb{T}(\mathcal{A})$  and then the row sum of  $(W|_{\mathbb{T}(\mathcal{A})})^{-1}$  at the row associated with  $t$  is positive, which implies the same is true for  $W^{-1}$ .

This also shows that if  $W|_{\mathbb{T}(\mathcal{A})}$  is a potential, so is  $W$ , proving the first part of (iv).



(iii) Now, we prove formula (2.1). Since  $W^{-1}$  is supported on  $\mathbb{T}$ , we have  $W_{ij}^{-1} = 0$  if  $d_{\mathbb{T}}(i, j) > 1$ . The inverse by blocks formula (5.1) and induction will show the result. If  $\mathbb{T}$  has cardinal 1 or 2, one checks easily the desired formula in this case. So we assume that  $\mathbb{T}$  has cardinal at least 3. In this situation if  $i, j$  are neighbors, then there exists a leaf  $t$  different from  $i, j$ . Denote  $\mathbb{L} = \mathbb{T} \setminus \{t\}$ , which is a tree.  $Z = W|_{\mathbb{L}}$  is again a Hadamard product of class one ultrametric matrices. Using Lemma 3.3 we can assume that this product is indexed by a subset of  $\mathbb{L}$ . So by induction, formula (2.1) holds for  $Z^{-1}$  and in particular this matrix is supported by  $\mathbb{L}$ . Therefore from (5.1), we get

$$W_{ij}^{-1} = Z_{ij}^{-1} = -\frac{W_{ij}}{W_{jj}W_{ii} - W_{ij}^2}$$

If  $d_{\mathbb{T}}(t, i) > 1$  and  $d_{\mathbb{T}}(t, j) > 1$ , we obtain again  $W_{ii}^{-1} = Z_{ii}^{-1}$  and  $W_{jj}^{-1} = Z_{jj}^{-1}$ , which proves the formula in this case.

The only extra instance to be analyzed is when  $d_{\mathbb{T}}(t, i) = 1 < d_{\mathbb{T}}(t, j)$  or  $d_{\mathbb{T}}(t, j) = 1 < d_{\mathbb{T}}(t, i)$ . Both situations are similar and we only consider the first one. In the notation of equation (5.1) we have  $s = i$ , and again  $W_{jj}^{-1} = Z_{jj}^{-1}$ . On the other hand  $W_{ii}^{-1} = Z_{ii}^{-1} + \alpha^2\theta$  which gives

$$W_{ii}^{-1} = \frac{1}{W_{ii}} + \sum_{k \in \mathbb{L}: d_{\mathbb{L}}(i, k)=1} \frac{W_{ki}^2}{W_{kk}W_{ii}^2 - W_{ki}^2W_{ii}} + \frac{W_{ti}^2}{W_{tt}W_{ii}^2 - W_{ti}^2W_{ii}}$$

proving the desired result.

(iv) Follows from formula (2.1).  $\square$

### 6. Matrices compatible with a tree

In the first part of this section we shall study some properties that are deduced from the hypothesis that the incidence graph for the inverse of a matrix is a tree. Then, we prove Theorem 2.4 and Theorem 2.5. In this section, we still denote  $i \sim j$  whenever  $(i, j) \in \mathbb{G}$  and  $i \neq j$ , even if  $\mathbb{G}$  is not a tree.

**Definition 6.1.** A matrix  $A$  with no zeroes in the diagonal is said to be **compatible** with the tree  $\mathbb{T}$  if

$$\forall i \sim j \quad A_{ij} \neq 0. \tag{6.1}$$

$$\forall i \sim j \quad A_{ii}A_{jj} - A_{ij}A_{ji} \neq 0. \tag{6.2}$$

For all  $i \sim j$  consider  $K = \{k : i \in \text{geod}_{\mathbb{T}}(k, j)\}$  and  $J = \{\ell : j \in \text{geod}_{\mathbb{T}}(\ell, i)\}$ , then

$$A_{KJ} = \frac{A_{ij}}{A_{ii}A_{jj}} A_{Ki}A_{jJ}, \quad A_{JK} = \frac{A_{ji}}{A_{ii}A_{jj}} A_{Jj}A_{iK}. \tag{6.3}$$

In what follows given a graph  $\mathbb{G}$ , we denote by  $\mathbb{G}^-$  the subgraph outside the diagonal.

**Lemma 6.2.** *Assume that  $A$  is compatible with the tree  $\mathbb{T}$ . Then,  $A$  is nonsingular,  $\mathbb{G}^-(A) = \mathbb{T}^-$  and formula (2.1) holds for  $A^{-1}$ , namely*

$$\begin{cases} A_{ii}^{-1} = \frac{1}{A_{ii}} \left( 1 + \sum_{t:\ell\sim i} \frac{A_{it}A_{ti}}{A_{tt}A_{ii}-A_{it}A_{ti}} \right), \\ A_{ij}^{-1} = -\frac{A_{ij}}{A_{jj}A_{ii}-A_{ij}A_{ji}}, \text{ if } i \sim j, \\ A_{ij}^{-1} = 0, \text{ if } i \neq j \text{ and } i \not\sim j. \end{cases} \tag{6.4}$$

**Proof.** Let  $B$  be the matrix given by the right hand side in (6.4). The result is proven as soon as we show that  $BA = \mathbb{I}$ . In what follows we denote  $\Delta_{ik} = A_{ii}A_{kk} - A_{ik}A_{ki}$ . We first compute

$$(BA)_{ii} = B_{ii}A_{ii} + \sum_{k\sim i} B_{ik}A_{ki} = 1 + \sum_{k\sim i} \frac{A_{ik}A_{ki}}{\Delta_{ik}} + \sum_{k\sim i} \frac{-A_{ik}}{\Delta_{ik}} A_{ki} = 1.$$

In order to show that  $(BA)_{i\ell} = 0$ , for  $\ell \neq i$ , we shall use more closely the compatibility relations of  $A$  and  $\mathbb{T}$ . Consider  $j \neq i$ , the unique neighbor of  $i$  in  $geod_{\mathbb{T}}(i, \ell)$  (if  $\ell \sim i$  then  $j = \ell$ ).

$$(BA)_{i\ell} = B_{ii}A_{i\ell} + B_{ij}A_{j\ell} + \sum_{k\sim i, k\neq j} B_{ik}A_{k\ell}.$$

From relation (6.3) in Definition 6.1, we have for  $k \sim i, k \neq j$

$$A_{k\ell} = \frac{A_{ki}}{A_{ii}} A_{i\ell}, \quad A_{i\ell} = \frac{A_{ij}}{A_{jj}} A_{j\ell}.$$

Hence,

$$\begin{aligned} (BA)_{i\ell} &= B_{ii}A_{i\ell} + B_{ij}A_{j\ell} + \frac{A_{i\ell}}{A_{ii}} \sum_{k\sim i, k\neq j} B_{ik}A_{ki} \\ &= B_{ii}A_{i\ell} + B_{ij}A_{j\ell} - \frac{A_{i\ell}}{A_{ii}} B_{ij}A_{ji} + \frac{A_{i\ell}}{A_{ii}} \sum_{k\sim i} B_{ik}A_{ki} \\ &= B_{ij}A_{j\ell} - \frac{A_{i\ell}}{A_{ii}} B_{ij}A_{ji} + \frac{A_{i\ell}}{A_{ii}} \left( B_{ii}A_{ii} + \sum_{k\sim i} B_{ik}A_{ki} \right) \\ &= B_{ij}A_{j\ell} - \frac{A_{i\ell}}{A_{ii}} B_{ij}A_{ji} + \frac{A_{i\ell}}{A_{ii}} = B_{ij}A_{j\ell} - \frac{A_{ij}A_{ji}}{A_{ii}A_{jj}} B_{ij}A_{j\ell} + \frac{A_{i\ell}}{A_{ii}} \\ &= \frac{-A_{ij}}{\Delta_{ij}} A_{j\ell} \left( 1 - \frac{A_{ij}A_{ji}}{A_{ii}A_{jj}} \right) + \frac{A_{i\ell}}{A_{ii}} = \frac{-A_{ij}A_{j\ell}}{A_{ii}A_{jj}} + \frac{A_{i\ell}}{A_{ii}} = 0 \end{aligned}$$

This shows the desired formula for  $A^{-1}$ .  $\square$

**Lemma 6.3.** *Assume that  $A$  is nonsingular and  $\mathbb{G}^-(A) = \mathbb{T}^-$ , where  $\mathbb{T}$  is a tree. We further assume that the diagonal elements of  $A$  are not 0. Then  $A$  is compatible with  $\mathbb{T}$ .*

**Proof.** We first assume the extra hypothesis that the diagonal of  $A^{-1}$  contains no zeroes, that is, for all  $t$  one has  $A_{tt}^{-1} \neq 0$ . At the end of the proof we remove this extra hypothesis by a perturbation argument. Let us start by showing property (6.3) in Definition 6.1.

If  $i \sim j$  then, after a permutation of rows and columns, the inverse of  $A$  has the form

$$H = \begin{pmatrix} \Gamma & A_{ij}^{-1} e_i f'_j \\ A_{ji}^{-1} f_j e'_i & \Omega \end{pmatrix}, \tag{6.5}$$

where  $e_i$  is the vector of size  $p = |K|$  with entries all 0, except the one associated with  $i \in K$ , which is a 1 (similarly for  $f_j$ , which has size  $q = |J|$ ). On the other hand  $\Gamma = A_{KK}^{-1}, \Omega = A_{JJ}^{-1}$ . Using that  $A_{ii}^{-1}$  is not zero, we can apply Gauss algorithm to reduce  $H$  to the form (in one iteration)

$$\tilde{H} = \begin{pmatrix} \Gamma & A_{ij}^{-1} e_i f'_j \\ 0 & \tilde{\Omega} \end{pmatrix},$$

showing that  $\Gamma$  is nonsingular. Similarly,  $\Omega$  is nonsingular too.

The inverse of  $H$ , which is a permutation of rows and columns of  $A$ , is

$$H^{-1} = \begin{pmatrix} D & E \\ F & G \end{pmatrix}.$$

Using the Schur’s complement we obtain that

$$F = A_{JK} = -A_{ji}^{-1} G f_j e'_i \Gamma^{-1} = uv',$$

where  $u = G f_j = A_{Jj} \in \mathbb{R}^p$  and  $v = -A_{ji}^{-1} (\Gamma^{-1})' e_i \in \mathbb{R}^q$ . Thus, we obtain for all  $\ell \in J, k \in K$  that  $A_{\ell k} = A_{\ell j} v_k$ . In particular we have  $A_{jk} = A_{jj} v_k$ , which implies that

$$A_{\ell k} = \frac{A_{\ell j}}{A_{jj}} A_{jk}. \tag{6.6}$$

Similarly, one has  $F = -A_{ji}^{-1} \Omega^{-1} f_j e'_i D = z(A_{iK})'$ , where  $z = -A_{ji}^{-1} \Omega^{-1} f_j$ . Thus,  $A_{hk} = z_h A_{ik}$  and therefore

$$A_{hk} = \frac{A_{hi}}{A_{ii}} A_{ik}.$$

Take  $j$  in place of  $h$  in this equality and replacing it in (6.6), we obtain  $A_{JK} = A_{Jj} \frac{A_{ji}}{A_{ii} A_{jj}} A_{iK}$ . The other part is shown similarly.

We shall prove (6.1) and (6.2) in Definition 6.1, using an inductive argument. We assume that both properties are true, whenever  $Z$  is a nonsingular matrix of order smaller or equal to  $n$ ,  $\mathbb{G}^-(Z)$  is a tree and the inverse of  $Z$  has no zeroes in the diagonal. For  $n = 1, 2$  both properties are straightforward to prove. So, assume that  $A$  is a nonsingular matrix of order  $n + 1 \geq 3$ ,  $\mathbb{G}^-(A) = \mathbb{T}^-$ , for some tree  $\mathbb{T}$ , and  $A^{-1}$  has no zeroes in the diagonal.

In what follows we fix  $s$  a leaf in  $\mathbb{T}$  and  $t$  the unique neighbor of  $s$ . We shall prove that  $\Delta_{st} \neq 0$ . From relation (6.3), we have for all  $\ell \neq s$  (notice that  $K = \{s\}$  and  $J = I \setminus \{s\}$ )

$$A_{s\ell} = \frac{A_{st}}{A_{tt}} A_{t\ell}.$$

So,  $A_{sJ} = \frac{A_{st}}{A_{tt}} A_{tJ}$  and if  $\Delta_{st} = 0$ , we obtain that  $A_{ss} = \frac{A_{st}}{A_{tt}} A_{ts}$ , proving that rows  $s, t$  are proportional, which is not possible. Hence  $\Delta_{st} \neq 0$ . On the other hand if  $A_{st} = 0$ , we conclude that  $A_{sJ} = 0$ , which implies that  $A$  has the block structure (after a permutation of rows and columns)

$$\begin{pmatrix} A_{ss} & 0 \\ A_{Js} & A_{JJ} \end{pmatrix}.$$

This shows that  $A_{st}^{-1} = 0$ , which is not possible, because  $s, t$  are neighbors in  $\mathbb{T}$ .

As in the first part of this proof, we consider the decomposition by blocks given by (6.5), where now  $\Gamma = A_{ss}^{-1}$ . Hence we obtain that

$$\tilde{\Omega} = \Omega - \frac{A_{st}^{-1} A_{ts}^{-1}}{A_{ss}^{-1}} f_t f_t' = (A^{-1})_{JJ} - \frac{A_{st}^{-1} A_{ts}^{-1}}{A_{ss}^{-1}} f_t f_t',$$

is nonsingular and supported by the tree  $\mathbb{L} = \mathbb{T} \setminus \{s\}$ . Its inverse is  $(\tilde{\Omega})^{-1} = A_{JJ} = G$ . The main problem for the induction is that  $\tilde{\Omega}_{tt}$  could be 0. So, we perturb this matrix by  $\epsilon$  in the diagonal and consider

$$\tilde{\Omega}(\epsilon) = \tilde{\Omega} + \epsilon \mathbb{I},$$

where  $\mathbb{I}$  is the identity of order  $n$ . Now, for small enough  $\epsilon > 0$ , this matrix is nonsingular, it is supported by  $\mathbb{L}$  and the diagonal elements are all nonzero. Thus we can apply the inductive argument to its inverse

$$G(\epsilon) = (\tilde{\Omega} + \epsilon \mathbb{I})^{-1} = G(\mathbb{I} + \epsilon G)^{-1} = G - \epsilon G^2 + \epsilon^2 G^3 - \dots$$

Notice also that for small  $\epsilon > 0$  the diagonal elements of  $G(\epsilon)$  are not 0. The induction shows that  $G(\epsilon)$  is compatible with  $\mathbb{L}$  and therefore we can apply formula (6.4) to  $G(\epsilon)$  to get for all  $k \sim l$  in  $\mathbb{L}$

$$\Delta_{kl}(\epsilon) G(\epsilon)_{kl} = -\tilde{\Omega}(\epsilon)_{kl} = -\tilde{\Omega}_{kl} = -\Omega_{kl} = -A_{kl}^{-1}.$$

Passing to the limit  $\epsilon \rightarrow 0$  we obtain

$$\Delta_{kl} A_{kl} = -A_{kl}^{-1} \neq 0,$$

because we have assumed that  $\mathbb{G}^-(A) = \mathbb{T}$ , which means that  $A_{kl}^{-1} \neq 0$ . This shows both properties (6.1) and (6.2) hold for  $G$  and then the same is true for  $A$ .

Now, we remove the extra hypotheses we have made by a similar perturbation argument as done before. For that purpose, consider  $\epsilon > 0$  small enough, such that  $A^{-1} + \epsilon \mathbb{I}$  is still nonsingular, and all the diagonal entries of this matrix are nonzero. We consider  $A(\epsilon) = (A^{-1} + \epsilon \mathbb{I})^{-1}$ , which is

$$A(\epsilon) = (A^{-1} + \epsilon \mathbb{I})^{-1} = A(\mathbb{I} + \epsilon A)^{-1} = A - \epsilon A^2 + \epsilon^2 A^3 - \dots$$

Notice that  $\mathbb{G}^-(A(\epsilon)) = \mathbb{G}^-(A) = \mathbb{T}^-$  and if we take  $\epsilon$  small enough, the diagonal elements of  $A(\epsilon)$  are not zero. Hence, (6.1) and (6.2) are satisfied for  $A(\epsilon)$ . Once again, formula (6.4) is valid for  $A(\epsilon)^{-1}$ . To finish the proof, it is enough to let  $\epsilon$  converge to 0.  $\square$

6.1. Proof of Theorem 2.4

Clearly (i)  $\Rightarrow$  (ii)  $\Rightarrow$  (iii). So, it is enough to show that (iii)  $\Rightarrow$  (i).

From formula (6.4) we have that  $A^{-1}$  is a Z-matrix. Since  $A$  is a positive matrix, we conclude that  $A^{-1}$  is an M-matrix.

Finally,  $A^{-1}$  is row diagonally dominant if and only if

$$A_{ii}^{-1} \geq \sum_{j \sim i} -A_{ij},$$

which is equivalent to (2.2) (see formula (6.4)). The proof is finished.  $\square$

6.2. Proof of Theorem 2.5

Assume that  $W$  is defined by Formula (2.4). If we interpret an empty product as 1, then the second case in the definition of  $W$  is a special case of the third. According to Lemma 6.2 and Theorem 2.4, the result is shown as soon as we prove that  $W$  is compatible with  $\mathbb{T}$ . Under the assumptions made on  $X$ , this is equivalent to proving that (6.3) holds for all  $i \sim j$ .

So, we take  $k \in K = \{\ell : i \in \text{geod}_{\mathbb{T}}(\ell, j)\}, t \in J = \{s : j \in \text{geod}_{\mathbb{T}}(s, i)\}$  and we compute  $W_{ks}$ . From the definition of  $W$  we get:

$$W_{ks} = \frac{W_{ki}}{W_{ii}} \frac{W_{ij}}{W_{jj}} W_{js},$$

and we obtain

$$W_{KJ} = \frac{W_{ij}}{W_{ii}W_{jj}} W_{Ki}W_{jJ}.$$

Similarly, we show that

$$W_{JK} = \frac{W_{ji}}{W_{ii}W_{jj}} W_{Jj}W_{iK},$$

and the result is shown.

Conversely, assume that  $W$  is an inverse  $M$ -matrix, with associated graph  $\mathbb{T}$ . The  $2 \times 2$  principal minors of an inverse  $M$ -matrix are always positive, so we only need to show that relation (2.4) holds. In a first place we assume that  $W$  is symmetric. So, we can use the multiplicative decomposition given in Theorem 2.1 (iii), to further reduce the problem to the case when  $W$  is a class 1 ultrametric matrix. We denote by  $r$  the root associated to  $W$ . Let  $i_0 = i, \dots, i_q = j$  be the geodesic in  $\mathbb{T}$  joining the different points  $i, j$ . We denote by  $i_s$ , the unique point in this geodesic closest to  $r$ . Then, ultrametricity shows that

$$\begin{aligned} W_{i_{p-1}, i_p} &= W_{i_p, i_p} = W_{i_s, i_s} = W_{ij} \quad \text{for } p = 1, \dots, s \\ W_{i_{p-1}, i_p} &= W_{i_{p-1}, i_{p-1}} \quad \text{for } p = s + 1, \dots, q. \end{aligned}$$

In particular, we have

$$W_{i_{q-1}, j} \prod_{p=1}^{q-1} \frac{W_{i_{p-1}, i_p}}{W_{i_p, i_p}} = W_{i_{q-1}, i_{q-1}} \prod_{p=s+1}^{q-1} \frac{W_{i_{p-1}, i_{p-1}}}{W_{i_p, i_p}} = W_{i_s, i_s} = W_{ij}.$$

This shows the result under the extra hypothesis that  $W$  is symmetric. Now, Theorem 2.1 (i) shows the existence of a diagonal matrix  $E$ , such that  $WE$  is a symmetric inverse  $M$ -matrix, associated to the same tree. The property holds for  $WE$  which shows that

$$W_{ij} E_{jj} = W_{i_{q-1}, j} E_{jj} \prod_{p=1}^{q-1} \frac{W_{i_{p-1}, i_p} E_{i_p, i_p}}{W_{i_p, i_p} E_{i_p, i_p}},$$

and the result is shown.  $\square$

**7. An algorithm: Proof of Theorem 2.7**

In this section we develop the algorithm we have proposed that determines whether a matrix is compatible with a tree. This algorithm gives necessary and sufficient conditions for a positive matrix, to be an inverse  $M$ -matrix supported on a tree. This together with condition (2.2) will give a characterization of potentials associated with random walks on trees. In what follows we assume that  $W$  is a positive matrix. Some of the results can be extended to more general situations, but we prefer to focus on the problem of characterizing potentials. So, if  $W$  is an inverse  $M$ -matrix, then  $\mathbb{G}(W)$  is connected.

Recall that given the matrix  $A$ , we associate the following symmetric matrix  $R = R(A)$

$$R_{ij} = \frac{A_{ij} A_{ji}}{A_{ii} A_{jj}}.$$

**Lemma 7.1.** *Assume that  $W$  is an inverse  $M$ -matrix and  $\mathbb{G}(A) = \mathbb{T}$  is a tree. Then  $R = R(W)$  satisfies:*

- (i) *For all  $i$  we have  $R_{ii} = 1$ , and for all  $i \neq j$   $0 < R_{ij} < 1$ ;*

(ii) if  $k \in \text{geod}_{\mathbb{T}}(i, j)$ , then

$$R_{ij} = R_{ik}R_{kj};$$

(iii) for  $i \neq j$  we have  $i \sim j$  if and only if  $R_{ij} > \max\{R_{ik}R_{kj} : k \neq i, j\}$ ;

(iv) assume that  $i \sim j$ , then  $i \in \text{geod}_{\mathbb{T}}(k, j)$  if and only if  $R_{ki} > R_{kj}$ .

**Remark 7.1.** Under the assumptions of the previous lemma, it can be proved that  $d(i, j) = -\log(R_{ij})$  is a distance in  $\mathbb{T}$  compatible with the tree structure. In particular, property (ii) simply reads as  $k \in \text{geod}_{\mathbb{T}}(i, j)$  then  $d(i, j) = d(i, k) + d(k, j)$ .

**Proof of Lemma 7.1.** First notice that there is a diagonal matrix  $F$  such that  $FW$  is a potential (this is a general result about inverse  $M$ -matrices see for example [13]). It is straightforward to show that  $R(FW) = R(W)$ . Since we also have  $\mathbb{G}(FW) = \mathbb{G}(W)$ , we can assume without loss of generality that  $W$  is a potential. We denote by  $X = (X_n : n \in \mathbb{N})$  the associated Markov chain and  $P$  its transition kernel.

(i). Since  $W_{ij} = \mathbb{P}_i(\tau_j < \infty)W_{jj}$ , we get for  $i \neq j$  that  $0 < R_{ij} = \mathbb{P}_i(\tau_j < \infty)\mathbb{P}_j(\tau_i < \infty) \leq 1$ . Let us prove that  $R_{ij} < 1$ . Since the Markov chain associated with  $W$  is transient, there must exist at least on node  $r$  that loses mass (a root):  $P_{rr} + \sum_{k \sim r} P_{rk} < 1$ .

One of the two alternatives must be true:  $j \in \text{geod}_{\mathbb{T}}(i, r)$  or  $i \in \text{geod}_{\mathbb{T}}(j, r)$ . In the former case  $\mathbb{P}_j(\tau_i < \infty) < 1$  because there is a path that connects  $j$  and  $r$  that does not visit  $i$ , namely  $\text{geod}_{\mathbb{T}}(j, r)$  and then

$$\mathbb{P}_j(\tau_i = \infty) \geq \mathbb{P}_j(\tau_r < \tau_i) \left( 1 - P_{rr} - \sum_{k \sim r} P_{rk} \right) > 0.$$

The other case is similar, and (i) is shown.

(ii). Assume that  $k \in \text{geod}_{\mathbb{T}}(i, j)$  and  $k \neq i, j$ , so, every path that connects  $i$  and  $j$  must pass through  $k$ . Then, the strong Markov property shows that

$$\mathbb{P}_i(\tau_j < \infty) = \mathbb{P}_i(\tau_k < \tau_j < \infty) = \mathbb{P}_i(\tau_k < \tau_j)\mathbb{P}_k(\tau_j < \infty) = \mathbb{P}_i(\tau_k < \infty)\mathbb{P}_k(\tau_j < \infty).$$

The last equality holds, because  $\tau_k < \tau_j$  is equivalent to  $\tau_k < \infty$  under  $\mathbb{P}_i$ . Similarly,

$$\mathbb{P}_j(\tau_i < \infty) = \mathbb{P}_j(\tau_k < \infty)\mathbb{P}_k(\tau_i < \infty),$$

which shows that  $R_{ij} = R_{ik}R_{kj}$ .

(iii). If  $i \neq j$  and  $R_{ij} > \max\{R_{ik}R_{kj} : k \neq i, j\}$ , then according to (ii) there cannot exist  $k \in \text{geod}_{\mathbb{T}}(i, j)$  different from  $i, j$ , that is  $i \sim j$ . Conversely, assume that  $i \sim j$ . Take any  $k \neq i, j$ . Without loss of generality we can assume  $j \in \text{geod}_{\mathbb{T}}(i, k)$ , which implies that  $R_{ik} = R_{ij}R_{jk}$  and therefore

$$R_{ik}R_{kj} = R_{ij}R_{kj}^2 < R_{ij},$$

because  $k \neq j$  implies  $R_{kj} < 1$ .

(iv). Assume that  $i \in \text{geod}_{\mathbb{T}}(k, j)$  then

$$R_{kj} = R_{ki}R_{ij} < R_{ki}.$$

On the other hand, assume that  $i \sim j$  and  $R_{kj} < R_{ki}$ . Then clearly  $k \neq j$ . If  $j \in \text{geod}_{\mathbb{T}}(k, i)$ , we obtain as before

$$R_{ki} < R_{kj},$$

which is a contradiction. Hence, since  $\mathbb{T}$  is a tree and  $i \sim j$ , we conclude that  $i \in \text{geod}_{\mathbb{T}}(k, j)$ . The result is shown.  $\square$

The following result is the basis for the algorithm we propose.

**Lemma 7.2.** *Assume  $A$  is a positive matrix and  $R = R(A)$ . We also assume that every  $2 \times 2$  principal minor of  $A$  is positive. The matrix  $A$  is compatible with a tree if and only if*

- (i) for all  $i$  there exists  $j$  such that  $i \overset{A}{\sim} j$ ;
- (ii) if  $i \overset{A}{\sim} j$  and if we denote  $K = \{k : R_{ki} > R_{kj}\}$ ,  $J = K^c$ , then

$$A_{KJ} = A_{Ki} \frac{A_{ij}}{A_{ii}A_{jj}} A_{jJ}, \quad A_{JK} = A_{Jj} \frac{A_{ji}}{A_{ii}A_{jj}} A_{iK}.$$

Moreover, a tree  $\mathbb{T}$  compatible with  $A$  is given by the relation  $\overset{A}{\sim}$ , that is, for  $i \neq j$  we have

$$(i, j) \in \mathbb{T} \Leftrightarrow i \overset{A}{\sim} j.$$

**Proof.** Assume first that  $A$  is compatible with the tree  $\mathbb{T}$ . Then from Lemma 6.2,  $A$  is nonsingular,  $\mathbb{G}^-(A) = \mathbb{T}^-$  (outside the diagonal) and formula (6.4) holds for the inverse. Then, since  $A > 0$  and every  $2 \times 2$  minor is also positive we conclude that  $A$  is an inverse  $M$ -matrix. Hence, the diagonal elements of  $A^{-1}$  are positive and then  $\mathbb{G}(A) = \mathbb{T}$ .

Now, we can apply Lemma 7.1 (iii) to conclude that  $i \overset{A}{\sim} j$  is equivalent to  $(i, j) \in \mathbb{T}$ , for all  $i \neq j$ , showing that (i) holds. From the definition of compatibility we deduce that for  $i \overset{A}{\sim} j$ , which is equivalent to  $i \sim j$  in  $\mathbb{T}$ , we obtain that

$$A_{KJ} = A_{Ki} \frac{A_{ij}}{A_{ii}A_{jj}} A_{jJ}, \quad A_{JK} = A_{Jj} \frac{A_{ji}}{A_{ii}A_{jj}} A_{iK},$$

where  $K = \{k : i \in \text{geod}_{\mathbb{T}}(k, j)\}$  and  $J = K^c$ . Part (ii) will follow as soon we prove that  $K = \{k : R_{ki} > R_{kj}\}$ . This is obtained from (iv) in Lemma 7.1 and the implication is proved.



Conversely, we assume that  $A$  is positive, that every  $2 \times 2$  minor is positive and (i), (ii) hold. We need to show that  $A$  is compatible with a tree. Actually, this is equivalent to showing that  $\overset{A}{\sim}$  is induced by a tree. We show this property by induction on  $n$ , the order of  $A$ .

The result is true when  $n = 1, 2$ . So, we assume it is true whenever the order of the matrix is smaller or equal to  $n$  and we show it holds true, when the order of  $A$  is  $n + 1 \geq 3$ . Let us denote  $I = \{1, \dots, n + 1\}$  and we fix some  $i \in I$ .

From part (i) there exists at least one  $j \neq i$  such that  $i \overset{A}{\sim} j$ . Since the minor  $A_{ii}A_{jj} - A_{ij}A_{ji} > 0$  we deduce that  $R_{ij} < 1 = R_{ii}$  and then  $K = \{k : R_{ki} > R_{kj}\}$  is not empty because it contains at least  $i$ . The same argument shows that  $J = K^c$  is not empty and contains at least  $j$ .

We claim that the matrices  $A_{KK}, A_{JJ}$ , which are of order at most  $n$ , satisfy the induction hypothesis. Let us show this is true for  $B = A_{KK}$ . Clearly, this matrix is positive and every  $2 \times 2$  principal minor is also positive. So, we prove it satisfies (i), (ii). First notice that  $R(B) = R_{KK}$ . Fix some  $\ell \in K$  and consider  $t \in K$  such that

$$R_{\ell t} = \max\{R_{\ell h} : h \in K \setminus \{\ell\}\}.$$

Then, for any  $h \in K \setminus \{\ell, t\}$  we have  $R_{\ell t} > R_{\ell h}R_{ht}$ , because  $R_{ht} < 1$ . This shows  $B$  satisfies (i).

Now, assume that  $\ell \overset{B}{\sim} t$ , of course for  $\ell, t \in K$ , that is

$$R_{\ell t} > \max\{R_{\ell s}R_{st} : s \in K \setminus \{\ell, t\}\}.$$

Using that  $A$  satisfies (ii), we have for all  $r \in I \setminus K$

$$R_{\ell r}R_{rt} = R_{\ell i}R_{ir}R_{ri}R_{it} = R_{\ell i}R_{it}R_{ir}^2 < R_{\ell i}R_{it} \leq R_{\ell t}.$$

The last inequality follows from the fact that  $i \in K$ . The equality holds only when  $\ell = i$  or  $t = i$ . Hence, we have proved that  $\ell \overset{A}{\sim} t$ . In particular by (ii) satisfied for  $A$ , we get

$$A_{LH} = A_{L\ell} \frac{A_{\ell t}}{A_{\ell\ell}A_{tt}} A_{tH}, \quad A_{HL} = A_{Ht} \frac{A_{t\ell}}{A_{\ell\ell}A_{tt}} A_{\ell L},$$

where  $L = \{s \in I : R_{s\ell} > R_{st}\}$  and  $H = I \setminus L$ . Now, let  $\tilde{L} = L \cap K = \{s \in K : R_{s\ell} > R_{st}\}$  and  $\tilde{H} = K \setminus \tilde{L} = K \cap H$ , then

$$B_{\tilde{L}\tilde{H}} = B_{\tilde{L}\ell} \frac{B_{\ell t}}{B_{\ell\ell}B_{tt}} B_{t\tilde{H}}, \quad B_{\tilde{H}\tilde{L}} = B_{\tilde{H}t} \frac{B_{t\ell}}{B_{\ell\ell}B_{tt}} B_{\ell\tilde{L}}.$$

This shows that  $B = A_{KK}$  satisfies the induction hypothesis. Then, there exists a tree  $\mathbb{L}_1$  such that for all  $\ell \neq t$  elements of  $K$

$$(\ell, t) \in \mathbb{L}_1 \Leftrightarrow \ell \overset{B}{\sim} t.$$

In order to prove that  $C = A_{JJ}$  also satisfies the induction hypothesis is enough to show that  $J = \{k : R_{ki} < R_{kj}\}$ . In order to show this representation for  $J$ , consider  $k \in J$  and then use (ii) satisfied by  $A$  to get

$$A_{ik} = \frac{A_{ij}}{A_{jj}} A_{jk}, \quad A_{ki} = \frac{A_{kj}}{A_{jj}} A_{ji}.$$

Hence,  $R_{ik} = R_{ij}R_{jk} < R_{jk}$  and the claim is shown.

The matrix  $C$  also satisfies the induction hypothesis and therefore there exists a tree  $\mathbb{L}_2$  such that for all  $r \neq s$  elements of  $J$

$$(r, s) \in \mathbb{L}_2 \Leftrightarrow r \overset{C}{\sim} s.$$

To finish the proof consider the tree  $\mathbb{T}$  which is obtained by joining  $\mathbb{L}_1, \mathbb{L}_2$  through the edge  $(i, j)$ . Let us show that  $\mathbb{T}$  is compatible with  $A$ , that is for all  $p \neq q$  in  $I$

$$(p, q) \in \mathbb{T} \Leftrightarrow p \overset{A}{\sim} q.$$

This is clear if  $p, q \in K$  or  $p, q \in J$ . So, the last case to consider is  $p \in K, q \in J$  and  $(p, q) \neq (i, j)$ . In this situation  $(p, q) \notin \mathbb{T}$ . On the other hand, if  $p \neq i$  we use that  $R_{pq} = R_{pi}R_{iq}$  to conclude that  $\neg(p \overset{A}{\sim} q)$ . If  $q \neq j$  the conclusion is similar. The result is shown.  $\square$

**Proof of Theorem 2.7.** The necessity of (i), (ii) follows from Lemma 6.3 and Lemma 7.2.

Conversely, assume conditions (i), (ii) hold. Then, according to Lemma 7.2 the matrix  $W$  is compatible with a tree. Now, from Lemma 6.2 we have  $W^{-1}$  is supported on that tree and formula (6.4) holds for  $W^{-1}$ , showing that  $W$  is an inverse  $M$ -matrix.  $\square$

### 8. Proof of Theorem 2.8

Properties (i), (iii), (iv) are shown as in Theorem 2.9 in [9]. The main tool we use is the existence of two diagonal matrices  $D, \widehat{D}$  such that  $U = DW\widehat{D}$  is a class 1 tree ultrametric matrix.

For part (ii) the main difficulty is to show that  $W^{(\alpha)}$  is nonsingular and its inverse is supported on  $\mathbb{T}$ . First notice that  $W^{(\alpha)} = (W^{(-\alpha)})^{(-1)}$  and  $W^{(-\alpha)}$  is an inverse  $M$ -matrix whose inverse is supported on  $\mathbb{T}$ . Thus, we can assume without loss of generality that  $\alpha = -1$ .

The matrix  $A = W^{(-1)}$  is a positive matrix. Each principal minor of order 2 is

$$\frac{1}{W_{ii}W_{jj}} - \frac{1}{W_{ij}W_{ji}} = \frac{W_{ij}W_{ji} - W_{ii}W_{jj}}{W_{ii}W_{jj}W_{ij}W_{ji}} < 0.$$

To conclude that  $A$  is compatible with  $\mathbb{T}$ , we assume that  $i \sim j$ . Using that  $W$  is compatible with  $\mathbb{T}$  we have

$$W_{KJ} = \frac{W_{ij}}{W_{ii}W_{jj}}W_{Ki}W_{jJ}, \quad W_{JK} = \frac{W_{ji}}{W_{ii}W_{jj}}W_{Jj}W_{iK},$$

where  $K = \{k \in \mathbb{T} : i \in \text{geod}_{\mathbb{T}}(k, j)\}$  and  $J = K^c$ . It is direct to show that

$$A_{KJ} = \frac{A_{ij}}{A_{ii}A_{jj}}A_{Ki}A_{jJ}, \quad A_{JK} = \frac{A_{ji}}{A_{ii}A_{jj}}A_{Jj}A_{iK}.$$

From Lemma 6.3 and formula (6.4), we conclude that  $A$  is nonsingular, its inverse satisfies (ii.2), that is the off diagonal elements of  $C = A^{-1}$  are nonnegative. Since  $A$  is a positive matrix then diagonal elements of  $C$  must be negative. Also,  $C$  is supported by  $\mathbb{T}$ .

Now we prove that  $\text{sign}(\det(A)) = (-1)^{n+1}$ . For that purpose we consider two positive diagonal matrices such that  $U = DWE$  is a class 1 tree ultrametric matrix. Obviously the sign of the determinant of  $U^{(-1)}$  and  $A$  is the same. So let us prove the claim for  $U^{(-1)}$ . This is done by induction and we suppose that the property is true for matrices of order smaller than  $n - 1 \geq 1$  and we show it for matrices of order  $n$ . Using a couple of extra diagonal matrices, we can assume that  $U$  has a unique root  $r$ , which is a leaf of  $\mathbb{T}$ . After a suitable permutation of rows and columns we can assume that  $U$  has a block structure as

$$U = \begin{pmatrix} U_{rr} & U_{rr}\mathbb{1}' \\ U_{rr}\mathbb{1} & V \end{pmatrix},$$

where  $\mathbb{1}$  is a vector of ones of size  $n - 1$  and  $V$  is a class 1 tree ultrametric matrix, supported by the tree  $\mathbb{L} = \mathbb{T} \setminus \{r\}$  and it has a unique root at  $s \in \mathbb{L}$ , the unique neighbor of  $r$  in  $\mathbb{T}$  (see Lemma 3.3). Notice that  $V_{s\bullet} = V_{ss}\mathbb{1}'$  and  $V_{ss} = U_{ss} > U_{rr}$ . Hence,

$$U^{(-1)} = \begin{pmatrix} 1/U_{rr} & 1/U_{rr}\mathbb{1}' \\ 1/U_{rr}\mathbb{1} & V^{(-1)} \end{pmatrix}.$$

To avoid any confusion we denote  $\Gamma = V^{(-1)}$ . Then,

$$\det(U^{(-1)}) = \frac{1}{U_{rr}} \left( 1 - \frac{1}{U_{rr}}\mathbb{1}'\Gamma^{-1}\mathbb{1} \right) \det(V^{(-1)}).$$

But, the structure of  $\Gamma = V^{(-1)}$  shows that  $\Gamma^{-1}\mathbb{1} = V_{ss}e_s = U_{ss}e_s$ . Therefore, we conclude that

$$1 - \frac{1}{U_{rr}}\mathbb{1}'\Gamma^{-1}\mathbb{1} = 1 - \frac{U_{ss}}{U_{rr}} < 0$$

and then  $\text{sign}(\det(U^{(-1)})) = -\text{sign}(\det(V^{(-1)}))$ , proving the claim.

The proof of (ii.3) follows from Cauchy’s Interlace Theorem for eigenvalues, the Perron–Frobenius Theorem and induction. For details see the proof of Theorem 2.9 in [9]. □

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**Appendix A. A decomposition for class 2 ultrametric matrices**

Consider  $U$  a class 2 ultrametric matrix with characteristic  $(\mathbb{T}, r, s, F, a)$ . We shall give an explicit possible decomposition  $U = V \odot Z$  where  $V, Z$  are class 1 ultrametric matrices. Recall that  $r, s$  are the roots of  $U$ . We can assume that the elements of  $U$  are greater than 1. For that, it is enough to multiply  $U$  by a large constant.

Also we assume that  $U$  has the block structure

$$U = \begin{pmatrix} A & a\mathbb{1}_p\mathbb{1}'_q \\ a\mathbb{1}_q\mathbb{1}'_p & B \end{pmatrix},$$

where  $A = U|_{\mathbb{T}_1}, B = U|_{\mathbb{T}_2}$ ,  $p$  and  $q$  are the sizes of trees  $\mathbb{T}_1 = \mathbb{T}_s[r], \mathbb{T}_2 = \mathbb{T}_r[s]$ . We also recall that  $A, B$  are nonsingular class 1 ultrametric matrices and  $a = U_{rs} < \min\{U_{rr}, U_{ss}\}$ . The root of  $A$  is  $r$  and the root of  $B$  is  $s$ , which in particular implies that  $\min\{A\} = U_{rr}, \min\{B\} = U_{ss}$ .

Now, we decompose  $V$  and  $Z$  similarly. We assume that  $V$  has a unique root at  $r$  and  $Z$  at  $s$

$$V = \begin{pmatrix} V_1 & V_{rr}\mathbb{1}_p\mathbb{1}'_q \\ V_{rr}\mathbb{1}_q\mathbb{1}'_p & V_2 \end{pmatrix}, \quad Z = \begin{pmatrix} Z_1 & Z_{ss}\mathbb{1}_p\mathbb{1}'_q \\ Z_{ss}\mathbb{1}_q\mathbb{1}'_p & Z_2 \end{pmatrix}.$$

We point out that  $V_{rr} = (V_1)_{rr} = \min\{V\}$  and similarly  $Z_{ss} = (Z_2)_{ss} = \min\{Z\}$ . We propose to search for a solution where  $V_1 = A^{(\alpha)}, Z_1 = A^{(1-\alpha)}$  and  $V_2 = B^{(\beta)}, Z_2 = B^{(1-\beta)}$ , with the restriction that  $0 < \alpha, \beta < 1$ .

The restrictions on these numbers are

$$\begin{aligned} V_{rr} &= U_{rr}^\alpha < U_{ss}^\beta = V_{ss}, \\ Z_{ss} &= U_{ss}^{1-\beta} < U_{rr}^{1-\alpha} = Z_{rr}, \\ a &= U_{rs} = V_{rr}Z_{ss} = U_{rr}^\alpha U_{ss}^{1-\beta}. \end{aligned}$$

If there is a solution to this problem, then it is straightforward to check that  $V, Z$  are class 1 ultrametric matrices, and  $U = V \odot Z$ . Without loss of generality we can assume that  $U_{rr} \leq U_{ss}$ . Then, the restrictions are

$$\begin{aligned} \alpha \frac{\log(U_{rr})}{\log(U_{ss})} &< \beta, \\ 1 - \frac{\log(U_{rr})}{\log(U_{ss})} + \alpha \frac{\log(U_{rr})}{\log(U_{ss})} &< \beta, \\ \beta &= \alpha \frac{\log(U_{rr})}{\log(U_{ss})} + 1 - \frac{\log(U_{rs})}{\log(U_{ss})}. \end{aligned}$$

It is straightforward to verify that for every  $0 < \alpha < 1$  there exists a solution to this problem (notice that  $U_{rs} < U_{rr} \leq U_{ss}$ ). So, there are infinite many ways to decompose  $U$ .

**Appendix B. An algorithm to compute  $\mathbb{T}$**

Here we propose an algorithm that decides when a positive matrix  $W$  has an inverse  $W^{-1}$ , which is an  $M$ -matrix supported on a tree. This algorithm is based on [Theorem 2.7](#) and [Theorem 2.5](#).

The first step is to compute  $R$ , which costs  $\frac{3}{2}n^2$  products and divisions.

**Step 0.** Set  $I_0 = I$ ,  $p_0 = n$  and

- (1)  $\forall i \in I_0 \left\{ \begin{array}{l} \mathcal{J}_0(i) = \min \left\{ j : j \in \operatorname{argmax} \{ R_{ik} : k \in I_0 \setminus \{i\} \} \right\}, \text{ check } R_{i \mathcal{J}_0(i)} < 1; \\ K_0(i) = \{ k \in I_0 : R_{ik} > R_{i \mathcal{J}_0(i)k} \}, \text{ compute } |K_0(i)|; \end{array} \right.$
- (2)  $\mathcal{L}_1 = \{ t : |K_0(t)| = 1 \}$ , set  $p_1 = |\mathcal{L}_1|$ , verify  $p_1 \geq 2$ ;
- (3)  $\forall i \in \mathcal{L}_1, k \in I_0, j = \mathcal{J}_0(i)$  verify that  $\begin{cases} W_{ik} = \frac{W_{ij}}{W_{jj}} W_{jk}; \\ W_{ki} = \frac{W_{ji}}{W_{jj}} W_{kj}. \end{cases}$
- (4)  $\forall i \in \mathcal{L}_1$  put  $(i, \mathcal{J}_0(i)) \in \mathbb{T}$ , and set  $I_1 = I_0 \setminus \mathcal{L}_1$ .

$\mathcal{L}_1$  is the set of leaves in case  $W^{-1}$  is supported on a tree. The cost for each subpart is: (1)  $2n^2$ , (2)  $n$ , (3)  $6p_1n$ , (4)  $3p_1$  (here we do not distinguish between products, divisions and sums). The total cost for step 0 is  $2n^2 + 6p_1n + n + 3p_1$ .

**Remark B.1.** An important property to verify is: For  $i \in \mathcal{L}_1$  one should have  $\mathcal{J}_0(i) \notin \mathcal{L}_1$  (unless  $n = 2$ ). Indeed, take  $k$  different from  $i$  and  $j = \mathcal{J}_0(i)$ . Then, from (3) we obtain

$$R_{ik} = \frac{W_{ik}W_{ki}}{W_{ii}W_{kk}} = \frac{W_{ij}W_{ji}}{W_{ii}W_{jj}} \frac{W_{jk}W_{kj}}{W_{jj}W_{kk}} = R_{ij}R_{jk} < R_{jk}, \tag{B.1}$$

because  $R_{ij} < 1$ . Now, assume that  $j \in \mathcal{L}_1$  and consider  $\ell = \mathcal{J}_0(j)$ . If  $\ell \neq i$  we get as above that  $R_{ij} = R_{ji} < R_{\ell i} = R_{i\ell}$ , contradicting the optimality of  $j$  in (1). Thus, the only possibility is that  $i = \mathcal{J}_0(j)$ , but then similarly to (B.1) we get

$$R_{jk} < R_{ik},$$

which is in contradiction with (B.1). The conclusion is that  $\mathcal{J}_0(i) \notin \mathcal{L}$ .

The next important observation is that if  $W^{-1}$  is an  $M$ -matrix supported on a tree  $\mathbb{T}$ , then  $(W_{I_1 I_1})^{-1}$  is again an  $M$ -matrix supported on  $\mathbb{T} \setminus \mathcal{L}_1$ . This allows us to proceed as follows.

**Step 1.**

- (1) define  $\widehat{\mathcal{L}}_2 = \{\mathcal{J}_0(i) : i \in \mathcal{L}_1\} \subseteq I_1$  (candidate set of leaves);
- (2)  $\forall i \in \widehat{\mathcal{L}}_2$  recompute  $\begin{cases} \mathcal{J}_1(i) = \min \{j : j \in \operatorname{argmax}\{R_{ik} : k \in I_1 \setminus \{i\}\}\}; \\ K_1(i) = \{k \in I_1 : R_{ik} > R_{\mathcal{J}_1(i)k}\}, \text{ compute } |K_1(i)|; \end{cases}$
- (3)  $\mathcal{L}_2 = \{i \in \widehat{\mathcal{L}}_2 : |K_1(i)| = 1\}$ , set  $p_2 = |\mathcal{L}_2|$ , verify  $p_2 \geq 2$ ;
- (4)  $\forall i \in \mathcal{L}_2, k \in I_1 \setminus \{i\}$ , with  $j = \mathcal{J}_1(i)$ , verify that  $\begin{cases} W_{ik} = \frac{W_{ij}}{W_{jj}} W_{jk}; \\ W_{ki} = \frac{W_{ji}}{W_{jj}} W_{kj}. \end{cases}$
- (5)  $\forall i \in \mathcal{L}_2$  put  $(i, \mathcal{J}_1(i)) \in \mathbb{T}$ , and set  $I_2 = I_1 \setminus \mathcal{L}_2$ .

The cost for this step is: (1)  $p_1$ , (2)  $3p_1(n - p_1)$ , (3)  $p_1$ , (4)  $6p_2(n - p_1)$ , (5)  $3p_2$  and the total cost for step 1 is

$$3(n - p_1)(p_1 + 2p_2) + 2p_1 + 3p_2.$$

Continue until step  $q$  for which

$$|I_q| \leq 1. \tag{B.2}$$

At this stage there are two possibilities. If  $|I_q| = 0$  then  $\mathcal{L}_q = I_{q-1}$ , with  $|I_{q-1}| \geq 2$ . According to Remark B.1 this is only possible if  $|I_{q-1}| = 2$ . Hence,  $p_q = 2, \sum_{m=1}^q p_m = n$  and the number of edges in  $\mathbb{T}$  is  $n - 1$ , because in step  $q - 1$  there are 2 nodes and 1 edge.

On the other hand, if  $|I_q| = 1$ , then  $|\mathcal{L}_q| = |I_{q-1}| - 1$  and  $\sum_{m=1}^q p_m = n - 1$ , which gives again  $n - 1$  edges.

Thus, if the algorithm stops at (B.2) it provides a graph  $\mathbb{T}$ , which has no cycles and it has  $n - 1$  edges, so it is a tree. To show that  $W$  is compatible with  $\mathbb{T}$  we use (2.4) in Theorem 2.5, that is, we need to show

$$W_{ik} = \left( \prod_{s=1}^{r-1} \frac{W_{i_{s-1}i_s}}{W_{i_s i_s}} \right) W_{i_{r-1}k},$$

where  $geod_{\mathbb{T}}(i, k) = \{i = i_0 \sim i_1 \sim \dots \sim i_{r-1} \sim i_r = k\}$  and  $r \geq 2$ . This property is proved using induction on the length of the geodesic between  $i$  and  $k$ .

Finally, the total cost of the algorithm is bounded by

$$\text{Cost} \leq \frac{3}{2}n^2 + 2n^2 + 6p_1n + n + 3p_1 + \sum_{\ell=1}^{q-1} 3(n - s_\ell)(p_\ell + 2p_{\ell+1}) + 2p_\ell + 3p_{\ell+1}$$

$$\begin{aligned} &\leq \frac{7}{2}n^2 + 6p_1n + n + 3n \sum_{\ell=1}^{q-1} p_\ell + 2p_{\ell+1} \leq \frac{7}{2}n^2 + 6(n-1)n + n + 9n^2 \\ &\leq \frac{37}{2}n^2, \end{aligned}$$

where  $s_\ell = \sum_{m=1}^{\ell} p_m$ .

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