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Description of the sub-Markov kernel associated to generalized ultrametric matrices. An algorithmic approach

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Abstract

We supply a simple algorithm which describes the sub-Markov kernel P associated to a nonsingular generalized ultrametric matrix U . This algorithm is based on the dyadic tree structure of U , it identifies the exiting roots of P and P^t , and the couples $i \neq j$ for which $P_{ij} > 0$ (equivalently $(U^{-1})_{ij} < 0$). © 2000 Elsevier Science Inc. All rights reserved.

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1. Introduction

Let I be a finite set and $U = (U_{ij}; i, j \in I)$ be a nonnegative matrix. Generalized ultrametric (GU) matrices and nested block form (NBF) matrices were introduced in [8,11]. After a suitable permutation, every GU matrix can be put in NBF. On the other hand, GU matrices generalize the notion of ultrametric matrices defined in [9]. Indeed, an ultrametric matrix is a symmetric GU matrix. Theorem 4.4 in [8] provides a remarkable criterion for the nonsingularity of a GU matrix U : U is

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nonsingular if and only if U does not contain a row of zeros and no two rows of U are the same (see also the criterion given in [11]: U is nonsingular if and only if $U + U^t$ is nonsingular). In the sequel, we assume U is a nonsingular GU matrix.

Theorem 4.4 in [8] and Theorem 3.6 in [11] state that $U^{-1} = ((U^{-1})_{ij}; i, j \in I)$ is a row and column diagonally dominant M-matrix (row and column DDM), i.e.

$$(U^{-1})_{ij} \leq 0 \quad \text{for } i \neq j \text{ in } I,$$

$$(U^{-1})_{ii} > 0 \quad \forall i \in I;$$

$$\sum_{j \in I} (U^{-1})_{ij} \geq 0 \quad \forall i \in I \quad (\text{row DD})$$

and

$$\sum_{j \in I} (U^{-1})_{ji} \geq 0 \quad \forall i \in I \quad (\text{column DD}).$$

This result generalizes the DDM property shown in [9] for ultrametric matrices. An algebraic proof of this last fact was given in [10].

The row DDM property implies that for every $\eta \geq \eta(U) := \max\{(U^{-1})_{ii} : i \in I\}$ the matrix $P := P^U$, depending on η and given by $P = (\mathbb{1} - \eta^{-1}U^{-1})$, is a sub-Markov kernel: $P_{ij} \geq 0 \forall i, j \in I$, $P\mathbf{1} \leq \mathbf{1}$ pointwise (where $\mathbb{1}$ is the identity matrix and $\mathbf{1}$ is the constant 1-vector). Therefore,

$$\eta U = (\mathbb{1} - P)^{-1} = \sum_{m \geq 0} P^m$$

and U is proportional to the potential matrix associated to the transient kernel P . Since $P_{ij} > 0 \Leftrightarrow U_{ij}^{-1} < 0$ for $i \neq j$, the existence of links between different points does not depend on η . On the other hand, the condition $P_{ii} > 0$ depends on the value of η .

In the theory of row DDM matrices, the main role is played by the *potential vector* $\mu := \mu_U$ associated to U by $\mu := U^{-1}\mathbf{1}$. From the row DDM property, μ is a nontrivial positive vector: $\mu_i \geq 0$ and its total mass $\bar{\mu} := \mathbf{1}^t\mu$ is strictly positive. Notice that the following equivalence holds:

$$\mu_i > 0 \Leftrightarrow (U^{-1}\mathbf{1})_i > 0 \Leftrightarrow (P\mathbf{1})_i < 1. \quad (1)$$

Every i satisfying this property is called an *exiting root of U* (or of P) and the set of them is denoted by $\mathcal{R} := \mathcal{R}_U$. The Markov chain defined by P loses mass at $i \in \mathcal{R}$. Since μ is nontrivial, \mathcal{R} is nonempty and P is strictly sub-Markovian.

For U , a row and column DDM matrix P is a double sub-Markov kernel, in particular $P^t\mathbf{1} \leq \mathbf{1}$. The potential vector $\nu := \nu_U$, associated to U^t , is given by $\nu := (U^t)^{-1}\mathbf{1}$ and its total mass by $\bar{\nu} := \mathbf{1}^t\nu$. Notice that $\bar{\mu} = \bar{\nu}$ because $\mathbf{1}^t\mu = (U^t\nu)^t\mu = \nu^t U\mu = \nu^t\mathbf{1}$. A relation similar to (1) holds for U^t . We define $\mathcal{R}^t := \mathcal{R}_{U^t}$ as the set of points, where the chain defined by P^t loses mass. We have $\mathcal{R}^t = \{i \in I : \nu_i > 0\}$ is nonempty and P^t is strictly sub-Markovian.

Our main results characterize, in an algorithmic way, the following properties (which do not depend on η): “ i is an exiting root of P ” and “for a given couple $i \neq j$, $P_{ij} > 0$ ”. These properties and other related problems were studied in [3] for the class of ultrametric matrices by means of a tree algorithm whose levels are given by the different values of the matrix. The methods we used in [3] for studying ultrametric matrices do not work, in general, for GU matrices.

In Section 2, we revisit GU matrices by means of dyadic filtrations, already used in [5] in the context of supermetric matrices. This idea is close to the one introduced in [11] for describing GU matrices. Theorem 1, stated and proved in Section 3, describes the exiting roots and associated sets for inverses of row DDM matrices. The rest of Section 3 is devoted to GU matrices, Theorems 2–4, where we characterize the exiting roots and the links of the sub-Markov kernel in terms of a graph algorithm. These results are proved in Sections 4 and 5. Our main tools are Schur’s decomposition, constancy sets along geodesics and Lemma 6, which provide a precise description on the disappearance of links. Theorem 5, in Section 6, describes the combinatorics of NBF matrices (permutations and filtrations). In Section 7, we revisit row DDM matrices in the framework of Markov chains and we prove some extra properties of GU matrices by probabilistic arguments.

We point out that since the pioneering work [2], ultrametricity has gained attention on matrix and operator theory (see for example [5,12,13] and references therein).

2. Generalized ultrametric

A *tree* (T, \mathcal{T}) is a finite nonoriented and connected graph, which does not contain nontrivial cycles of length greater than or equal to 3. For $(t, s) \in T \times T$, $t \neq s$, there is a unique path $\text{geod}(t, s)$ of minimum length, which is called the geodesic between t and s . We put $\text{geod}(t, t) = \{t\}$, which is of length 0. We fix $t^* \in T$ and we call it the *tree root* of T . If $s \in \text{geod}(t, t^*)$, we denote $s \leq t$, which is a partial order relation on T . For $t, s \in T$, $t \wedge s = \sup\{v \in \text{geod}(t, t^*) \cap \text{geod}(s, t^*)\}$ denotes the closest common ancestor of s and t . For every $t \neq t^*$, there exists a unique element in T , called the *predecessor* of t , denoted by $\mathbf{p}(t)$, which satisfies: $\mathbf{p}(t) < t$, and $(\mathbf{p}(t), t) \in \mathcal{T}$. The set of successors of t is $\mathbf{s}(t) = \{s \in T: s > t, (s, t) \in \mathcal{T}\}$. $I(\mathcal{T}) = \{i \in T: \mathbf{s}(i) = \emptyset\}$ is the set of leaves of the tree. The tree is said to be *dyadic* if $|\mathbf{s}(t)| = 2$ for $t \notin I(\mathcal{T})$. For $t \notin I(\mathcal{T})$, the successors are denoted by t^- and t^+ , the signs $-$ and $+$ are fixed once and for all in a dyadic tree. We also denote by t', t'' the successors of t when we do not want to precise their sign.

For $t \in T$, the set $L(t) := \{i \in I(\mathcal{T}): t \in \text{geod}(i, t^*)\}$ characterizes t . Then, we can identify t and $L(t)$, in particular t^* is identified with $L(t^*) = I(\mathcal{T})$ and $i \in I(\mathcal{T})$ with the singleton $\{i\}$. Hence, we can assume that each node of T is a subset of the set of leaves $I(\mathcal{T})$. The distinction between the roles of L , as $L \in T$ and $L \subseteq I$, will be clear in the context we use them.

We define GU matrices by using similar concepts as those introduced in relations (2.4) and (2.5) of [11].

Definition 1. $U = (U_{ij}: i, j \in I)$ is a GU matrix if there exist a dyadic tree (T, \mathcal{T}) and positive real vectors $\vec{\alpha} = (\alpha_t: t \in T)$, $\vec{\beta} = (\beta_t: t \in T)$ satisfying

- (a) $I = I(\mathcal{T})$, $\vec{\alpha}|_I = \vec{\beta}|_I$;
- (b) $\alpha_t \leq \beta_t$ for $t \in T$;
- (c) $\vec{\alpha}$ and $\vec{\beta}$ are \leq -increasing, i.e. $t \leq s$ implies $\alpha_t \leq \alpha_s$ and $\beta_t \leq \beta_s$;
- (d) $U_{ij} = \alpha_t$ if $(i, j) \in t^- \times t^+$ and $U_{ij} = \beta_t$ if $(i, j) \in t^+ \times t^-$, where $t = i \wedge j$;
- (e) $U_{ii} = \alpha_i = \beta_i$ for $i \in I$.

We will say that (T, \mathcal{T}) supports U .

The proof that this definition is equivalent to Definition 2.4 in [8] or to Definition 2.3 in [11] is given in Theorem 3.3 in [11]. The main point is that the symmetric matrices $U^1 = (U_{ij}^1 = \alpha_{i \wedge j})$ and $U^2 = (U_{ij}^2 = \beta_{i \wedge j})$ are ultrametric matrices, and the same tree can be associated to each of them. In this framework, ultrametric matrices are those GU matrices with $\vec{\alpha} = \vec{\beta}$.

Observe that for every $L \in T$ the matrix $U_L := U|_{L \times L}$ is also GU. The tree supporting it, denoted by (T_L, \mathcal{T}_L) , is the restriction of (T, \mathcal{T}) on the subtree originated at L , and the associated vectors are the restrictions of $\vec{\alpha}$ and $\vec{\beta}$ on T_L . The potential vectors and the exiting roots of U_L , U_L^t are denoted, respectively, by $\mu_L, \nu_L, \mathcal{R}_L, \mathcal{R}_L^t$. If U is a nonsingular GU matrix and $L \in T$, Schur's decomposition and an inductive argument show that U_L is also a nonsingular GU matrix. Therefore, all our results obtained for U will also apply for U_L .

We now introduce the following relation $\leq_{\mathcal{T}}$ in the set of leaves I ,

$$\text{for } i \neq j, \quad \text{we put } i <_{\mathcal{T}} j \quad \text{if } i \in t^-, \quad j \in t^+ \quad \text{with } t = i \wedge j. \tag{2}$$

It is easy to see that $\leq_{\mathcal{T}}$ is a total order in I . A set $Y \subseteq I$ is called a $\leq_{\mathcal{T}}$ -interval if $[i \leq_{\mathcal{T}} k \leq_{\mathcal{T}} j \text{ and } i, j \in Y] \Rightarrow k \in Y$. Clearly every element $L \in T$ is a $\leq_{\mathcal{T}}$ -interval.

Assume that $I = \{1, \dots, n\}$. By permuting I we can suppose $\leq_{\mathcal{T}}$ is the usual order relation \leq on I (i.e. $i + 1$ is the successor of i with respect to $\leq_{\mathcal{T}}$). For $i < j$, we have $i \wedge j = i \wedge i + 1 \wedge \dots \wedge j$. Therefore, from the \leq -increasing property of $\vec{\alpha}, \vec{\beta}$ we get

$$U_{ij} = \begin{cases} \min\{\alpha_{i \wedge i+1}, \dots, \alpha_{j-1 \wedge j}\} & \text{if } i < j, \\ \min\{\beta_{j \wedge j+1}, \dots, \beta_{i-1 \wedge i}\} & \text{if } i > j. \end{cases}$$

Observe that there exists i_0 satisfying $i_0 \wedge (i_0 + 1) = t^* = I$. Then,

$$\alpha_{i_0 \wedge i_0+1} = \alpha_I = \min\{\alpha_{i \wedge i+1}: i = 1, \dots, n - 1\} = \min\{U_{ij}: i, j \in I\},$$

$$\beta_{i_0 \wedge i_0+1} = \beta_I = \min\{\beta_{i \wedge i+1}: i = 1, \dots, n - 1\} = \min\{U_{ij}: i \geq j\}.$$

This situation takes place at all levels of the tree. We will assume that this is the standard presentation of the GU matrix U , called an NBF. A more precise discussion is developed in Section 5.

Let us partition $I = I^- \cup I^+$ and denote $J := I^-$, $K := I^+$. The NBF implies that $U_{J \times K} = \alpha_I \mathbf{1}_J \mathbf{1}_K^t$, $U_{K \times J} = \beta_I \mathbf{1}_K \mathbf{1}_J^t$ and

$$U = \begin{bmatrix} U_J & \alpha_I \mathbf{1}_J \mathbf{1}_K^t \\ \beta_I \mathbf{1}_K \mathbf{1}_J^t & U_K \end{bmatrix},$$

where U_J, U_K are also nonsingular matrices in NBF. Denote

$$U^{-1} = \begin{bmatrix} C & D \\ E & F \end{bmatrix}.$$

By Schur’s decomposition one obtains

$$\begin{aligned} C &= U_J^{-1} + \frac{\alpha_I \beta_I \bar{\mu}_K}{1 - \alpha_I \beta_I \bar{\mu}_J \bar{\mu}_K} \mu_J v_J^t, & E &= -\frac{\beta_I}{1 - \alpha_I \beta_I \bar{\mu}_J \bar{\mu}_K} \mu_K v_J^t, \\ D &= -\frac{\alpha_I}{1 - \alpha_I \beta_I \bar{\mu}_J \bar{\mu}_K} \mu_J v_K^t, & F &= U_K^{-1} + \frac{\alpha_I \beta_I \bar{\mu}_J}{1 - \alpha_I \beta_I \bar{\mu}_J \bar{\mu}_K} \mu_K v_K^t. \end{aligned} \tag{3}$$

These equations constitute the basic tool for our analysis.

3. Main results

We begin by studying the set of exiting roots of U . Theorem 1 below has a probabilistic meaning, as it will be stated in Section 7. In this way, part (a) asserts that the point minimizing the mean absorption time is an exiting root of U . The rest of this Theorem is devoted to analyze the sets

$$\mathcal{H}_r = \{j \in I : U_{jr} = U_{rr}\} \text{ defined for } r \in \mathcal{R}.$$

In the sequel, we use the notation $\operatorname{argmin}\{i \in I : Z_i\}$ for the set of points minimizing Z .

Theorem 1. *Let U be the inverse of a row DDM matrix.*

- (a) $\operatorname{argmin}\{i \in I : \sum_{j \in I} U_{ij}\} \subseteq \mathcal{R}$;
- (b) $(\mathcal{H}_r : r \in \mathcal{R})$ are disjoint;
- (c) For $r \in \mathcal{R}$: $\mathcal{H}_r \cap \mathcal{R} = \{r\}$ and $[j \in \mathcal{H}_r, j \neq r, s \notin \mathcal{H}_r \Rightarrow (U^{-1})_{js} = 0]$.

Proof. (a) Take $i_0 \in \operatorname{argmin}\{i \in I : \sum_{j \in I} U_{ij}\}$. From the equality $U^{-1}U = \mathbb{1}$, we obtain $\sum_{\ell \in I} \sum_{j \in I} (U^{-1})_{i_0 \ell} U_{\ell j} = 1$. For $\ell \neq i_0$, we have $(U^{-1})_{i_0 \ell} \leq 0$. Then, the minimal condition on i_0 implies $\sum_{j \in I} U_{i_0 j} \sum_{\ell \in I} (U^{-1})_{i_0 \ell} \geq 1$, from which $\sum_{\ell \in I} (U^{-1})_{i_0 \ell} > 0$. Hence, i_0 is an exiting root. As a by-product we have obtained the lower bound $\mu_{i_0} \geq (\sum_{j \in I} U_{i_0 j})^{-1}$.

(c) Let us take $j \in \mathcal{H}_r, j \neq r$. Therefore, $\sum_{s \in I} (U^{-1})_{js} U_{sr} = 0$ or equivalently $U_{rr} \sum_{s \in \mathcal{H}_r} (U^{-1})_{js} = -\sum_{s \in I \setminus \mathcal{H}_r} (U^{-1})_{js} U_{sr}$. Since all the off-diagonal elements of U^{-1} are nonpositive, we get $-\sum_{s \in I \setminus \mathcal{H}_r} (U^{-1})_{js} \geq 0$. If this last sum were strictly positive, we shall arrive at the inequality

$$U_{rr} \sum_{s \in \mathcal{H}_r} (U^{-1})_{js} < -U_{rr} \sum_{s \in I \setminus \mathcal{H}_r} (U^{-1})_{js},$$

because for $s \in I \setminus \mathcal{H}_r$ we have $U_{sr} < U_{rr}$. Then, $U_{rr} \sum_{s \in I} (U^{-1})_{js} < 0$, which contradicts the fact that U^{-1} is a row DD matrix. We conclude

$$(U^{-1})_{js} = 0 \text{ for every } s \notin \mathcal{H}_r \text{ and } \sum_{s \in \mathcal{H}_r} (U^{-1})_{js} = 0,$$

in particular $j \notin \mathcal{R}$, which proves (c).

(b) Let r, r' be two different exiting roots. From (c), one obtains $r \notin \mathcal{H}_{r'}$ and $r' \notin \mathcal{H}_r$. Assume that $j \in \mathcal{H}_r \cap \mathcal{H}_{r'}$. Then $r \neq j \neq r'$. From (c) we also get that $(U^{-1})_{js} < 0$ implies $s \in \mathcal{H}_r \cap \mathcal{H}_{r'}$. Since $U = \eta^{-1} \sum_{m \geq 0} P^m$ and $U_{jr} = U_{rr} > 0$, there exists $m \geq 1$ satisfying $P_{jr}^{(m)} > 0$. Consider

$$m_0 = \min \left\{ m \geq 1 : P_{\ell r}^{(m)} > 0 \text{ and } \ell \in \mathcal{H}_r \cap \mathcal{H}_{r'} \right\},$$

and let $j_0 \in \mathcal{H}_r \cap \mathcal{H}_{r'}$ be some optimal site for the above minimization problem. In case $m_0 \geq 2$, we obtain

$$0 < P_{j_0 r}^{(m_0)} = \sum_{s \in I} P_{j_0 s} P_{sr}^{(m_0-1)}.$$

However, this last sum vanishes because $P_{j_0 s} > 0$ only if $s \in \mathcal{H}_r \cap \mathcal{H}_{r'}$ and then, by the definition of m_0 , $P_{sr}^{(m_0-1)} = 0$. This is a contradiction and we are left with the case $m_0 = 1$. Hence, $P_{j_0 r} > 0$ or equivalently $(U^{-1})_{j_0 r} < 0$, and then $r \in \mathcal{H}_r \cap \mathcal{H}_{r'}$. This is also a contradiction and the result is proved. \square

Remark 1. We point out that in case there is a unique root r , then $\mathcal{H}_r = I$ as is proved in the last section using probabilistic arguments.

We pursue with the idea of the previous proof to get an algorithm for detecting all the exiting roots in the context of a GU matrix, which is based on the block structure of these matrices.

For convenience, whenever we need to select a point $i_0 \in \operatorname{argmin}\{i \in I : Z_i\}$ we take the smallest one.

Theorem 2. Let U be a nonsingular GU matrix.

(a) The set of exiting roots \mathcal{R} is given by the following algorithm. Initially we put $I_0 = I$, $\mathcal{R}_{-1} = \emptyset$ and $k = 0$.

$$\text{Step } k: \begin{cases} i_k \in \operatorname{argmin}\{i \in I_k : \sum_{j \in I} U_{ij}\}, \\ H_k = \{j \in I_k : U_{ji_k} = U_{i_k i_k}\}, \\ \mathcal{R}_k = \mathcal{R}_{k-1} \cup \{i_k\}, \quad I_{k+1} = I_k \setminus H_k. \end{cases}$$

If $I_{k+1} = \emptyset$, then $\mathcal{R} = \mathcal{R}_k$ and we stop. Otherwise, we continue with step $k + 1$.

(b) $\mathcal{H}_r = H_k$ if $r = i_k$, ($\mathcal{H}_r : r \in \mathcal{R}$) is a partition of I and every \mathcal{H}_r is a $\leq_{\mathcal{F}}$ -interval.

Remark 2.

- (a) For the inverse of a row DDM matrix, the algorithm provided in Theorem 2 does not work in general. Even though the family $(\mathcal{H}_r: r \in \mathcal{R})$ is disjoint (after Theorem 1(b)), these sets do not necessarily cover I . In fact, consider a sub-Markov kernel P with at least two different exiting roots r_1, r_2 and an extra point $i \notin \mathcal{R}$ and verifying $P_{ir_1} > 0, P_{ir_2} > 0$. Then, by Theorem 1, $i \notin \bigcup_{r \in \mathcal{R}} \mathcal{H}_r$.
- (b) For GU matrices, even if the sets \mathcal{H}_r are intervals, they are not necessarily elements of T . For instance, take $I = \{1, 2, 3\}$ and consider the GU matrix

$$U = \begin{bmatrix} \gamma & \delta & \xi \\ \chi & \chi & \xi \\ \chi & \chi & \gamma \end{bmatrix},$$

where $\gamma > \chi > \delta > \xi > 0$. We have $T = \{\{1, 2, 3\}, \{1, 2\}, \{1\}, \{2\}, \{3\}\}, \leq_{\mathcal{T}}$ is the usual order in $I, \mathcal{R} = \{1, 2\}$ and $\mathcal{H}_2 = \{2, 3\} \notin T$.

Let us introduce the following subsets (recall $\alpha_i = \beta_i$ for a leaf $i \in I$):

$$\mathcal{N}_i^+ = \{L \in T: L \leq i, \alpha_L = \alpha_i\} \quad \text{and} \quad \mathcal{N}_i^- = \{L \in T: L \leq i, \beta_L = \beta_i\}.$$

Since $\vec{\alpha}$ is increasing in (T, \leq) , \mathcal{N}_i^+ is the set of constancy of $\vec{\alpha}$ starting from the leaf i (similarly for $\vec{\beta}$ and \mathcal{N}_i^-). This means

$$L \in \mathcal{N}_i^- \text{ (respectively } \mathcal{N}_i^+) \\ \text{implies } \text{geod}(i, L) \subseteq \mathcal{N}_i^- \text{ (respectively } \mathcal{N}_i^+).$$

In particular, if $L \in \mathcal{N}_i^-$ (respectively \mathcal{N}_i^+), $L \neq \{i\}$, then L^- or L^+ belongs to \mathcal{N}_i^- (respectively \mathcal{N}_i^+).

Since $\alpha_i = \beta_i \geq \beta_L \geq \alpha_L$, if $\alpha_L = \alpha_i$, then $\alpha_L = \beta_L = \beta_i = \alpha_i$. Hence, $\forall i \in I: \mathcal{N}_i^+ \subseteq \mathcal{N}_i^-$.

Recall the notation of successors $\mathbf{s}(L) = \{L', L''\}$. We construct the following sets of (forbidden) nonoriented arcs $\Gamma \subseteq \mathcal{T}, \Gamma^t \subseteq \mathcal{T}$:

$$\begin{aligned} (L, L') \in \Gamma &\Leftrightarrow \exists i \in L'' \text{ such that} \\ &\quad \{[L' = L^- \Rightarrow L \in \mathcal{N}_i^+] \text{ and } [L' = L^+ \Rightarrow L \in \mathcal{N}_i^-]\}, \\ (L, L') \in \Gamma^t &\Leftrightarrow \exists i \in L'' \text{ such that} \\ &\quad \{[L' = L^- \Rightarrow L \in \mathcal{N}_i^-] \text{ and } [L' = L^+ \Rightarrow L \in \mathcal{N}_i^+]\}. \end{aligned} \tag{4}$$

Theorem 3. *Let U be a nonsingular GU matrix, $L \in T$ and $i \in L$. Then $i \in \mathcal{R}_L \Leftrightarrow \text{geod}(i, L) \cap \Gamma = \emptyset$ and $i \in \mathcal{R}_L^t \Leftrightarrow \text{geod}(i, L) \cap \Gamma^t = \emptyset$.*

As a consequence of this theorem, we get the following characterization of the conservation of exiting roots. For $L' \in \mathbf{s}(L)$

$$\mathcal{R}_{L'} \subseteq \mathcal{R}_L \Leftrightarrow (L, L') \notin \Gamma.$$

In the next result, we describe exactly the links of P out of the diagonal. It is established in terms of roots which we are able to recognize because of previous theorems.

Theorem 4. *Let U be a nonsingular GU matrix. Let $i \neq j \in I$, $L = i \wedge j$, $\mathbf{s}(L) = \{L', L''\}$, with $i \in L'$ and $j \in L''$. Then*

- (a) $P_{ij}^L > 0 \Leftrightarrow i \in \mathcal{R}_{L'}$ and $j \in \mathcal{R}_{L''}$;
- (b) $P_{ij} > 0 \Leftrightarrow P_{ij}^L > 0$ and one (and only one) of the following two conditions is satisfied:
 - (b1) $U_{ij} = \beta_{i \wedge j} > \alpha_{i \wedge j}$;
 - (b2) $U_{ij} = \alpha_{i \wedge j}$ and for every $M < i \wedge j$ such that $\alpha_M = \alpha_{i \wedge j}$ it holds

$$[\{i, j\} \subseteq M^- \Rightarrow (M, M^-) \notin \Gamma^t] \quad \text{and} \quad [\{i, j\} \subseteq M^+ \Rightarrow (M, M^+) \notin \Gamma].$$

Part (a) is a consequence of Schur’s decomposition and follows directly from relation (3). The deeper part of Theorem 4 is (b) which characterizes when a connection at some level L pursues until the coarsest level I .

Corollary 1. *If $U_{ii} > \sup\{U_{ij}, U_{ji} : j \neq i\}$ for all $i \in I$, then $\mathcal{R} = \mathcal{R}^t = I$ and $P_{ij} > 0$ for every couple $i \neq j$.*

Proof. It is sufficient to notice that in this case Γ and Γ^t are empty. \square

Example 1. Let $\gamma < \delta < \xi$, $I = \{1, \dots, 6\}$. Consider the following matrix $U = (U_{ij} : i, j \in I)$:

$$U = \begin{bmatrix} \delta & \gamma & \gamma & \gamma & \gamma & \gamma \\ \delta & \xi & \gamma & \gamma & \gamma & \gamma \\ \delta & \delta & \delta & \gamma & \gamma & \gamma \\ \delta & \delta & \delta & \xi & \delta & \delta \\ \delta & \delta & \delta & \delta & \delta & \delta \\ \delta & \delta & \delta & \delta & \delta & \xi \end{bmatrix}.$$

In Fig. 1, at the left-hand side, we display a dyadic tree supporting its GU structure, \mathcal{T} being the set of arrows between the nodes of the tree. At the right-hand side, we display the nonoriented graph $\mathcal{T} \setminus \Gamma$. In this example, $\alpha_J = \gamma, \beta_J = \delta, \alpha_K = \delta, \beta_K = \delta, J^- = L, J^+ = \{3\}, 1 \wedge 3 = J, \mathcal{N}_1^- = \{1, L, J, I\}, \mathcal{N}_5^+ = \{5, M, K\}$. From Theorem 3 we have $\mathcal{R} = \{1\}, \mathcal{R}_K = \{5\}, 1 \in \mathcal{R}_{J^-}, 3 \in \mathcal{R}_{J^+}$. From Theorem 4(a), we get $P_{13}^J > 0$. On the other hand, $(I, J) \in \Gamma^t$ because $I \in \mathcal{N}_5^-, 5 \in K$. Since $U_{ij} = \alpha_{i \wedge j} = \alpha_I$, we deduce from Theorem 4(b2) that $P_{13} = 0$.

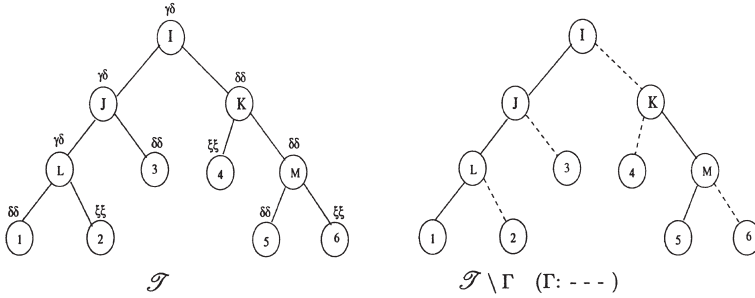


Fig. 1.

4. Proof of Theorems 2 and 3

In the sequel, we will denote by $U_{\bullet j}$ the j th column of U and by $U_{i\bullet}$ its i th row. This notation is also used for U_L . We assume that U is in NBF.

The following result follows from Theorem 3.6 in [8].

Lemma 1.

- (a) $\alpha_I \bar{\mu} \leq 1$ and $\beta_I \bar{\mu} \leq 1$.
- (b) $\alpha_I \bar{\mu} = 1$ iff $\exists!$ $j_0 \in I$ such that $U_{\bullet j_0} = \alpha_I \mathbf{1}$ and $U_{j_0 \bullet} = \alpha_I \mathbf{1}^t$. Moreover, $\beta_I = \alpha_I$ and $\mu = \nu = \alpha_I^{-1} \delta_{j_0}$ (where $(\delta_{j_0})_i = 1$ if $i = j_0$ and $= 0$ otherwise).
- (c) $\beta_I \bar{\mu} = 1$ implies $U_{nj} = \beta_I \forall j \in \mathcal{R}$.

The following lemma, whose proof is based on Schur’s decomposition, relates the exiting roots of U_J, U_K, U , as well as their potential vectors, where $J = I^-$, $K = I^+$.

Lemma 2. *The quantity $\Delta := 1 - \alpha_I \beta_I \bar{\mu}_J \bar{\mu}_K$ is strictly positive, and the potential vectors are related by*

$$\mu = \begin{bmatrix} a\mu_J \\ b\mu_K \end{bmatrix}, \quad \nu = \begin{bmatrix} cv_J \\ dv_K \end{bmatrix} \tag{5}$$

with

$$\begin{aligned} a &= \Delta^{-1}(1 - \alpha_I \bar{\mu}_K), & b &= \Delta^{-1}(1 - \beta_I \bar{\mu}_J), \\ c &= \Delta^{-1}(1 - \beta_I \bar{\mu}_K), & d &= \Delta^{-1}(1 - \alpha_I \bar{\mu}_J). \end{aligned} \tag{6}$$

Moreover,

$$\begin{aligned} \mathcal{R} &= \mathcal{R}_J \cup \mathcal{R}_K \text{ iff } [\alpha_I \bar{\mu}_K < 1 \text{ and } \beta_I \bar{\mu}_J < 1], \\ \mathcal{R} &= \mathcal{R}_J \text{ iff } \beta_I \bar{\mu}_J = 1 \text{ and } \mathcal{R} = \mathcal{R}_K \text{ iff } \alpha_I \bar{\mu}_K = 1. \end{aligned} \tag{7}$$

An analogous statement holds for the exiting roots of U^t .

Proof. The equations $U\mu = \mathbf{1}$, $U^t\nu = \mathbf{1}$ have unique solutions, and we shall prove that these solutions are given by (5) and (6). The systems for the unknown a, b, c, d are

$$\begin{aligned} a + \alpha_I \bar{\mu}_K b &= 1, & c + \beta_I \bar{\mu}_K d &= 1, \\ a \beta_I \bar{\mu}_J + b &= 1, & c \alpha_I \bar{\mu}_J + d &= 1. \end{aligned}$$

The determinant of both equations is Δ . Since $\beta_I \bar{\mu}_J \leq 1$ and $\beta_I \bar{\mu}_K \leq 1$, we get that $\Delta = 0$ implies $\alpha_I \bar{\mu}_J = 1$ and $\alpha_I \bar{\mu}_K = 1$. Therefore, $\alpha_I = \beta_I$ and both matrices U_J, U_K have a constant line equal to α_I , which implies U has two equal lines, contradicting the nonsingularity of U . Relation (7) follows directly. \square

Lemma 3.

- (a) $\alpha_I \bar{\mu} = 1$ iff [$\alpha_I \bar{\mu}_J = 1$ or $\alpha_I \bar{\mu}_K = 1$]. In the first case, $j_0 \in J$ and in the second one, $j_0 \in K$ (where j_0 is the index of Lemma 1(b)).
- (b) $\beta_I \bar{\mu} = 1$ iff [$\beta_I \bar{\mu}_J = 1$ or $\beta_I \bar{\mu}_K = 1$]. In the first case, $U_{mj} = \beta_I \forall j \in \mathcal{R}_J$ (where $m = |J|$) and in the second one, $U_{nj} = \beta_I \forall j \in \mathcal{R}_K$.

Proof. (a) Follows at once from Lemma 1.

(b) We only prove the equivalence because the rest follows from Lemma 1(c). We have

$$\beta_I \bar{\mu} = \beta_I(a\bar{\mu}_J + b\bar{\mu}_K) = \frac{\beta_I}{\Delta}(\bar{\mu}_J + \bar{\mu}_K - (\alpha_I + \beta_I)\bar{\mu}_J\bar{\mu}_K).$$

A simple computation gives

$$\beta_I \bar{\mu} \leq 1 \text{ is equivalent to } (1 - \beta_I \bar{\mu}_J)(1 - \beta_I \bar{\mu}_K) \geq 0,$$

with the equality being satisfied simultaneously on both sides. Then the equivalence is shown. \square

As mentioned before, the results already obtained, even if they are formulated for I , the first level of the tree, can be applied for every node $L \in T$.

Lemma 4.

- (a) $\alpha_L \bar{\mu}_L = 1$ if and only if $L \in \mathcal{N}_i^+$ for some leaf $i \in L$. In this case, $\beta_L = \alpha_L = \alpha_i = \beta_i$.
- (b) $\beta_L \bar{\mu}_L = 1$ if and only if $L \in \mathcal{N}_i^-$ for some leaf $i \in L$. In this case, $\beta_L = \beta_i$.

Proof. For part (a), we must show that there exists a leaf $i \in L$ such that $\alpha_i = \alpha_L$. From Lemma 1(b), $\alpha_L \bar{\mu}_L = 1$ iff there exists a column $i \in L$ such that $(U_L)_{\bullet i} = \alpha_L \mathbf{1}_L$ and $U_{ii} = \alpha_i = \alpha_L$. Reciprocally, assume that $\alpha_i = \alpha_L$ for $i \in L$. Since $U_{ii} = \alpha_i = \alpha_L$, we conclude the result. The equality $\beta_L = \alpha_L = \alpha_i$ follows from Lemma 1(b).

We now turn to the proof of (b). If L is a leaf, the result follows at once. Otherwise, we must show that there exists a leaf $i \in L$ such that $\beta_L = \beta_i$. We deduce from Lemma 3 that for some $L' \in \mathfrak{s}(L)$, we must have $\beta_L \bar{\mu}_{L'} = 1$. Since $\beta_{L'} \geq \beta_L$ and $\beta_{L'} \bar{\mu}_{L'} \leq 1$, we deduce $\beta_{L'} = \beta_L$. By recurrence we show that the condition is necessary. The condition is also sufficient because $\beta_L = \beta_i$ for some leaf $i \in L$ implies $\beta_M = \beta_L \forall M \in \text{geod}(i, L)$. Then, by Lemma 3 and recurrence, it follows that $\beta_M \bar{\mu}_M = 1 \forall M \in \text{geod}(i, L)$. \square

Proof of Theorem 2. We reason by induction on n . Notice that if $U_{i^*i^*} = \alpha_I$ for some $i^* \in I$, which is necessarily unique, then in the algorithm $i_0 = i^*$, $I_0 = I$, $I_1 = \emptyset$. Hence $\mathcal{R} = \{i_0\}$, and the result is shown in this case. Therefore, in the sequel, we can assume $U_{ii} > \alpha_I$ for every $i \in I$.

(a) We prove that the algorithm supplies the exiting roots of U .

(a1) First consider the case $U_{ii} > \beta_I$ for all $i \in J$. For every step k in the algorithm, we have

$$[i_k \in J \Rightarrow H_k \subset J] \quad \text{and} \quad [i_k \in K \Rightarrow H_k \subset K]. \tag{8}$$

In fact, if $i_k \in J$ and $j \in K$, we have $U_{ji_k} = \beta_I < U_{i_k i_k}$, and if $i_k \in K$ and $j \in J$, we get $U_{ji_k} = \alpha_I < U_{i_k i_k}$.

According to Lemmas 2 and 4(b) $\mathcal{R} = \mathcal{R}_J \cup \mathcal{R}_K$. We can assume, by an inductive argument, that our algorithm works for matrices U_J and U_K : $\mathcal{R}_J = \{i_0^J, \dots, i_p^J\}$ and $\mathcal{R}_K = \{i_0^K, \dots, i_q^K\}$. We denote by H_k^J, J_k, H_k^K, K_k the corresponding sets obtained when applying the algorithm to U_J and U_K .

Denote by k_0, \dots, k_l the steps at which the algorithm applied to the matrix U gives nodes i_{k_0}, \dots, i_{k_l} in J . We now prove that $l = p$ and $(i_{k_0}, \dots, i_{k_p}) = (i_0^J, \dots, i_p^J)$. Using (8) we get $J \subseteq I_{k_0}$. Since $\sum_{\ell \in J} (U_J)_{i\ell} + \alpha_I |K| = \sum_{\ell \in I} U_{i\ell}$ for every $i \in J$, we obtain that $i_0^J = i_{k_0}$, so $H_0^J = H_{k_0}, J_1 = I_{k_0+1} \cap J, I_{k_0+1} \cap K = I_{k_0} \cap K$. Another inductive argument shows the desired relation $l = p$ and $(i_{k_0}, \dots, i_{k_p}) = (i_0^J, \dots, i_p^J)$. We can argue similarly for matrix U_K , and hence, $\mathcal{R} = \mathcal{R}_J \cup \mathcal{R}_K$.

(a2) We are left with the case $U_{i^*i^*} = \beta_I$ for some $i^* \in J$ (notice that from the GU property this is the complementary of the above case). From Lemmas 2 and 4(b), $\mathcal{R} = \mathcal{R}_J$. Then we must show that our algorithm supplies this result. Notice that in this case $\alpha_I < \beta_I$. Then

$$\text{for every } j \in K \quad \text{we have} \quad \sum_{\ell \in I} U_{i^*\ell} \leq \beta_I |J| + \alpha_I |K| < \sum_{\ell \in I} U_{j\ell}.$$

Since (H_k) is clearly a partition of I , there exists a step m such that $i^* \in H_m$. We assume that i^* is optimal in the sense that $U_{i^*i^*} = \beta_I$ and m is the smallest possible value. We necessarily have $i_0, \dots, i_m \in J, H_k \cap K = \emptyset$ for every $k < m$, and $U_{i^*i_m} = U_{i_m i_m}$. Now

$$\beta_I = U_{i^*i^*} \geq U_{i^*i_m} = U_{i_m i_m} \geq \beta_I.$$

Then $U_{i_m i_m} = \beta_I = U_{j i_m}$ for every $j \in K$. We deduce $H_m = H_m^J \cup K$, and hence the algorithm supplies the equality $\mathcal{R} = \mathcal{R}_J$.

(b) Notice that $H_k \subseteq \mathcal{H}_r$ for $r = i_k$. Since (H_k) covers I , so does (\mathcal{H}_r) . Theorem 1 ensures that (\mathcal{H}_r) is a disjoint family proving that it is a partition. We also deduce that $H_k = \mathcal{H}_r$ for $r = i_k$.

Let us prove that for every $r \in \mathcal{R}$, \mathcal{H}_r is an interval. Observe that $i \leq_{\mathcal{J}} j \leq_{\mathcal{J}} k$ implies

$$U_{ik} \leq U_{jk} \leq U_{kk} \quad \text{and} \quad U_{ii} \geq U_{ij} \geq U_{ik}.$$

Let $i \in \mathcal{H}_r$. If $i \leq_{\mathcal{J}} j \leq_{\mathcal{J}} r$, then $U_{rr} = U_{ir} \leq U_{jr} \leq U_{rr}$ and we conclude $j \in \mathcal{H}_r$. Analogously if $r \leq_{\mathcal{J}} j \leq_{\mathcal{J}} k$. \square

Proof of Theorem 3. We only prove the part concerning \mathcal{R}_L , the other one is entirely analogous. Let $M \in \mathbf{s}(L)$. From Lemmas 3 and 4, the set of links Γ given in (4) can be described as follows:

$$(L, M) \in \Gamma \quad \text{iff} \quad [M = L^-, \alpha_L \bar{\mu}_{L^+} = 1 \text{ or } M = L^+, \beta_L \bar{\mu}_{L^-} = 1]. \quad (9)$$

For $i \in L$, denote $\text{geod}(i, L) = (L_0 = \{i\}, L_1, \dots, L_\ell = L)$. From (7) we have $i \in \mathcal{R}_L$ if and only if $i \in \mathcal{R}_{L_k}$ for every $k = 0, \dots, \ell$. The result is proved by recurrence on ℓ with the help of (9) and (7). \square

We pursue with the study of Γ in order to give a graphical description of \mathcal{H}_r for $r \in \mathcal{R}$.

Lemma 5. Let $\mathbf{s}(L) = \{L', L''\}$. Then $(L, L') \in \Gamma$ iff there exists a unique $i \in \mathcal{R}_{L''}$ such that

$$[L' = L^- \Rightarrow L \in \mathcal{N}_i^+] \quad \text{and} \quad [L' = L^+ \Rightarrow L \in \mathcal{N}_i^-]. \quad (10)$$

Proof. If $L' = L^-$, then from Lemma 1(b) and (9) there exists a unique $i \in \mathcal{R}_{L''}$ satisfying (10). Hence, in the rest of the proof we assume $L' = L^+$. We first prove the existence.

By definition, $(L, L') \in \Gamma$ if there exists $k \in L''$ satisfying (10). By an inductive argument it suffices to show that if $\ell \in \mathcal{R}_{M'}$ for some $M' \succ L''$ but $\ell \notin \mathcal{R}_M$ for $M = \mathbf{p}(M')$, then there exists $j \in M''$ satisfying (10). In fact, if $M' = M^+$, since $\ell \in \mathcal{R}_{M'} \setminus \mathcal{R}_M$, then necessarily exists $j \in M^-$ such that $\beta_M = \beta_j$. Hence $\beta_M = \beta_j = \beta_L$ and $L \in \mathcal{N}_j^-$. If $M' = M^-$, then there exists $j \in M^+$ such that $\alpha_M = \alpha_j = \beta_j$. So $\beta_L = \beta_M = \alpha_M = \beta_j$ and $L \in \mathcal{N}_j^-$.

Let us show the uniqueness. Consider $i, j \in \mathcal{R}_{L''}$ to be two different elements satisfying (10). Let $M = i \wedge j$, which satisfies $M \succeq L''$. Given that $L' = L^+$, we have $\beta_L = \beta_M = \beta_i = \beta_j$, and no element of \mathcal{R}_{M^+} belongs to \mathcal{R}_M . Since $i \in \mathcal{R}_{M^+}$ or $j \in \mathcal{R}_{M^+}$, one of the two elements does not belong to \mathcal{R}_M , contradicting $\mathcal{R}_{L''} \cap M \subseteq \mathcal{R}_M$. \square

We put $j \sqsubset i$ if $i \in \mathcal{R}_{L^c}$, $j \in \mathcal{R}_L$ and (10) is satisfied by L^c and i (i eliminates j from the set of exiting roots). Denote by $\widetilde{\sqsubset}$ the transitive and reflexive closure of \sqsubset . Observe that $r \in \mathcal{R}$, if and only if r is $\widetilde{\sqsubset}$ -maximal, i.e. $[r \widetilde{\sqsubset} j \Rightarrow r = j]$.

Proposition 1. For $r \in \mathcal{R}$, we have $\mathcal{H}_r = \{j \in I: j \widetilde{\sqsubset} r\}$.

Proof. Let $j \sqsubset i$ and $L = i \wedge j$. If $j \in L^-$, then $U_{ij} = \alpha_{i \wedge j} = \alpha_L = \alpha_i = U_{ii}$ and, if $j \in L^+$, then $U_{ij} = \beta_{i \wedge j} = \beta_L = \beta_i = U_{ii}$. In particular, if $j \sqsubset r$, then $j \in \mathcal{H}_r$. If $k \widetilde{\sqsubset} j \sqsubset r$, we have $j \wedge r = k \wedge r$, then $U_{kr} = U_{jr} = U_{rr}$, from which $k \in \mathcal{H}_r$. Therefore, $\{j \in I: j \widetilde{\sqsubset} r\} \subseteq \mathcal{H}_r$. Now, if $k \widetilde{\sqsubset} r$ is not satisfied and $r \in \mathcal{R}$, we can directly show that $U_{kr} \neq U_{rr}$. Also this can be proved by the fact that $(\mathcal{H}_r: r \in \mathcal{R})$ and $(\{j \in I: j \widetilde{\sqsubset} r\}: r \in \mathcal{R})$ are both partitions of I (the last one by construction, the first one from Theorem 2) and $\{j \in I: j \widetilde{\sqsubset} r\} \subseteq \mathcal{H}_r$. \square

5. Proof of Theorem 4

From (3), every $(i, j) \in J \times K \cup K \times J$ satisfies

$$(U^{-1})_{ij} < 0 \text{ if and only if } (i, j) \in \mathcal{R}_J \times \mathcal{R}_K^t \cup \mathcal{R}_K \times \mathcal{R}_J^t.$$

Then Theorem 4(a) follows.

Previously to show Theorem 4(b) it will be useful to supply some elementary properties. Consider $U(\gamma) = U - \gamma \mathbf{1}\mathbf{1}^t$. Observe that $\alpha_I \bar{\mu} < 1$ is equivalent to $\alpha_I < \min\{U_{ii}: i \in I\}$. Under this condition, for all $\gamma \in [0, \alpha_I]$ we get

$$U(\gamma)^{-1} = U^{-1} + \frac{\gamma}{1 - \gamma \bar{\mu}} \mu v^t. \tag{11}$$

By direct computations, we find that the potential vectors of $U(\gamma)$ and $U(\gamma)^t$ satisfy

$$\mu_{U(\gamma)} = \frac{1}{1 - \gamma \bar{\mu}} \mu, \quad v_{U(\gamma)} = \frac{1}{1 - \gamma \bar{\mu}} v. \tag{12}$$

For our analysis we will need the following key lemma.

Lemma 6. Let $\gamma \in [0, \alpha_I]$ and $\gamma < \min\{U_{ii}: i \in I\}$. Then, for $i \neq j$:

$$U_{ij} > \gamma \Rightarrow [(U^{-1})_{ij} < 0 \Leftrightarrow (U(\gamma)^{-1})_{ij} < 0], \tag{13}$$

$$U_{ij} = \gamma \Rightarrow (U(\gamma)^{-1})_{ij} = 0. \tag{14}$$

Proof. From hypothesis, the GU matrix $U(\gamma)$ is nonsingular because its diagonal is strictly positive and no two rows are equal. Denote by $P(\gamma)$ a sub-Markovian matrix such that $U(\gamma) = \eta^{-1} \sum_{m \geq 0} P(\gamma)^m$ for some $\eta > 0$. For $i \neq j$ we have $(P(\gamma))_{ij} = 0$ if and only if $(U(\gamma)^{-1})_{ij} = 0$. Since $(U(\gamma))_{ij} = 0$ implies $(P(\gamma))_{ij} = 0$, relation (14) is satisfied.

Let us prove (13). Assume $i \neq j$, $U_{ij} > \gamma$. From (11) and since $\gamma \geq 0$, we get that $(U(\gamma)^{-1})_{ij} < 0$ implies $(U^{-1})_{ij} < 0$. We now prove the reciprocal. Thus, we assume $(U^{-1})_{ij} < 0$, and split the proof into two cases.

Case $\gamma < \alpha_I$. If $(U(\gamma)^{-1})_{ij} = 0$, we arrive at a contradiction because $(U(\gamma)^{-1})_{ij}$ is increasing in the set $\{\gamma \leq \alpha_I\}$. Then we are able to find some $\gamma' < \alpha_I$ such that $(U(\gamma')^{-1})_{ij} > 0$ which contradicts that $U(\gamma')^{-1}$ has nonpositive off-diagonal elements.

Case $\gamma = \alpha_I$. By hypothesis $\alpha_I \bar{\mu} < 1$. Then $\alpha_I \bar{\mu}_J < 1$ and $\alpha_I \bar{\mu}_K < 1$. Hence,

$$U(\alpha_I) = \begin{bmatrix} U_J(\alpha_I) & 0 \\ (\beta_I - \alpha_I)\mathbf{1}_K \mathbf{1}_J^t & U_K(\alpha_I) \end{bmatrix}$$

and

$$U(\alpha_I)^{-1} = \begin{bmatrix} U_J(\alpha_I)^{-1} & 0 \\ \hat{E} & U_K(\alpha_I)^{-1} \end{bmatrix}.$$

In the case $(i, j) \in J \times J$, we get $(U(\alpha_I)^{-1})_{ij} = (U_J(\alpha_I)^{-1})_{ij}$. From (3), $(U_J^{-1})_{ij} \leq (U^{-1})_{ij} < 0$ and we obtain the result by induction on the dimension of the matrix. The argument when $(i, j) \in K \times K$ is similar. Therefore, we can assume $i \in K$, $j \in J$. Since $(U(\alpha_I))_{ij} > 0$, we have $\beta_I > \alpha_I$. From (3), we obtain $\hat{E} = -(\beta_I - \alpha_I)\mu_K(\alpha_I)v_J^t(\alpha_I)$, where $\mu_K(\alpha_I)$ and $v_J(\alpha_I)$ are, respectively, the potentials of matrices $U_K(\alpha_I)$ and $U_J(\alpha_I)^t$. To finish the proof we must show the equivalence of $E_{ij} < 0 \Leftrightarrow \hat{E}_{ij} < 0$. Since $E = -(\beta_I/\Delta)\mu_K v_J^t$, we conclude the result from (12) because

$$\mu_K(\alpha_I) = \frac{1}{1 - \alpha_I \bar{\mu}_K} \mu_K, \quad v_J(\alpha_I) = \frac{1}{1 - \alpha_I \bar{\mu}_J} v_J. \quad \square$$

Lemma 7. For $i \neq j$ in J we have

$$\alpha_I \bar{\mu}_J = 1 \Rightarrow (U^{-1})_{ij} = (U_J^{-1})_{ij}, \tag{15}$$

$$(U^{-1})_{ij} = 0 \Leftrightarrow (U_J^{-1})_{ij} = 0 \text{ or } [U_{ij} = \alpha_I \text{ and } \beta_I \bar{\mu}_K = 1]. \tag{16}$$

Proof. From (3) we have

$$(U^{-1})_J = U_J^{-1} + \frac{\gamma}{1 - \gamma \bar{\mu}_J} \mu_J v_J^t = U_J(\gamma)^{-1}$$

with $\gamma = \alpha_I \beta_I \bar{\mu}_K \leq \alpha_I \leq \min\{(U_J)_{ij}; i, j \in J\}$.

Assume that $\alpha_I \bar{\mu}_J = 1$. Then, we obtain $\alpha_I = \beta_I$ and $\mu_J = v_J = \alpha_I^{-1} \delta_{j_0}$ for some $j_0 \in J$, from which (15) follows.

We now turn to the proof of equivalence (16). From $(U_J^{-1})_{ij} \leq (U^{-1})_{ij} \leq 0$ we get $(U_J^{-1})_{ij} = 0 \Rightarrow (U^{-1})_{ij} = 0$. Thus, for the rest of the proof we may assume $(U_J^{-1})_{ij} < 0$ and we must show the following equivalence:

$$(U^{-1})_{ij} = 0 \Leftrightarrow [U_{ij} = \alpha_I \text{ and } \beta_I \bar{\mu}_K = 1].$$

Consider first the case $\alpha_I \bar{\mu}_J = 1$. Hence, from (15) $(U^{-1})_{ij} = (U_J^{-1})_{ij} < 0$. Since $\Delta = 1 - \alpha_I \bar{\mu}_J \beta_I \bar{\mu}_K > 0$, one obtains $\beta_I \bar{\mu}_K < 1$, proving in this case the equivalence.

Finally, we assume that $\alpha_I \bar{\mu}_J < 1$. Since $\gamma \leq \alpha_I < \min\{(U_J)_{ii} : i \in J\}$, we can apply Lemma 6 to the matrix U_J . If $(U_J)_{ij} = U_{ij} = \alpha_I$ and $\beta_I \bar{\mu}_K = 1$, we are in the case $(U_J)_{ij} = \gamma$. Hence $(U^{-1})_{ij} = (U_J(\gamma)^{-1})_{ij} = 0$. On the contrary, if $U_{ij} > \alpha_I$ or $\beta_I \bar{\mu}_K < 1$, we are in the case $(U_J)_{ij} > \gamma$, which implies $(U_J(\gamma)^{-1})_{ij} < 0 \Leftrightarrow (U_J^{-1})_{ij} < 0$, from which the result follows. \square

We now furnish the proof of Theorem 4(b). Since (b1) and (b2) cannot be satisfied simultaneously and clearly $P_{ij} > 0 \Rightarrow P_{ij}^L > 0$, we are reduced to prove the equivalent statement: under $P_{ij}^L > 0$, the equivalence $P_{ij} > 0 \Leftrightarrow$ (b1) or (b2), holds. Relation (16) in Lemma 7 shows that under condition (b1) one gets $P_{ij} > 0$. Assume now that (b1) is not satisfied, that is $U_{ij} = \alpha_L$, and consider $M < L$ such that $\alpha_M = \alpha_L$. Denote $s(M) = \{M', M''\}$ with $\{i, j\} \subseteq M'$. From Lemma 7, we get that $P_{ij}^M > 0 \Leftrightarrow [P_{ij}^{M'} > 0 \text{ and } \beta_M \mu_{M''} < 1]$. Using Lemma 2, $\beta_M \mu_{M''} < 1$ is equivalent to

$$[M' = M^- \Rightarrow \mathcal{R}_{M'}^t \subseteq \mathcal{R}_M^t] \text{ and } [M' = M^+ \Rightarrow \mathcal{R}_{M'} \subseteq \mathcal{R}_M].$$

From Theorem 3, we get this statement is equivalent to

$$[M' = M^- \Rightarrow (M, M^-) \notin \Gamma^t] \text{ and } [M' = M^+ \Rightarrow (M, M^+) \notin \Gamma],$$

proving the result by an inductive argument. \square

6. Combinatoric aspects of nested block form matrices

The purpose of this section is to describe some combinatorial aspects of the NBF matrices introduced in Definition 2.8 in [8] and Theorems 3.2 and 3.3 in [11]. In Section 3, we have shown that a GU matrix can be put in NBF after a suitable permutation. In Theorem 5(a) below, we will describe the set of permutations preserving the NBF structure of a matrix. We provide a criterion in terms of the tree supporting the matrix, or equivalently in terms of the associated sequence of partitions.

The elements of a partition ω of $I = \{1, \dots, n\}$ are called atoms; they are disjoint, nonempty and cover I . We denote by $\underline{\omega} = \{I\}$ the trivial partition and by $\bar{\omega} = \{\{i\} : i \in I\}$ the discrete one. We say ω' partitions dyadically ω , we put $\omega \prec^d \omega'$, if every atom of ω which is not a singleton is partitioned into two atoms in ω' . We call $\mathcal{F} = (\omega_0 \prec^d \dots \prec^d \omega_r)$ a *dyadic filtration* (of partitions) of I , and if $\omega_0 = \underline{\omega}$ and $\omega_r = \bar{\omega}$, \mathcal{F} is said to be a *total dyadic filtration*. We associate to the dyadic tree (T, \mathcal{F}) the total dyadic filtration $\mathcal{F} = (\omega_0 \prec^d \dots \prec^d \omega_r)$, where ω_{k+1} is formed from ω_k by partitioning all the atoms L in ω_k which are not singletons, into L^- and L^+ in ω_{k+1} . Reciprocally, associated to a total dyadic filtration \mathcal{F} we construct the following dyadic tree (T, \mathcal{F}) (below \subset means strict inclusion):

$$T = \bigcup_{k=0}^r \bigcup_{L \in \omega_k} \{L\} \quad \text{and} \quad \mathcal{F} = \{(L, J): L \in \omega_k, J \in \omega_{k+1}, J \subset L\},$$

and with tree root equal to I . In the definition below, we assume that I is endowed with the standard order.

Definition 2. The nonnegative matrix $U = (U_{ij}: i, j \in I)$ is in NBF if the vectors $\vec{a}, \vec{b} \in \mathbb{R}^{n-1}$ defined by $a_i = U_{i,i+1}, b_i = U_{i+1,i}$ $i = 1, \dots, n - 1$, satisfy the following conditions:

- (a) $a_i \leq b_i$ $i = 1, \dots, n - 1$;
- (b) $U_{ii} \geq \max\{b_{i-1}, b_i\}$, where for convenience $b_0 = 0, b_n = U_{nn}$;
- (c) $U_{ij} = \min\{a_i, \dots, a_{j-1}\}$ if $i < j, U_{ij} = \min\{b_j, \dots, b_{i-1}\}$ if $i > j$;
- (d) The following algorithm starting from the trivial partition $\omega_0 = \underline{\omega}$ at step $k = 0$ stops at the discrete partition $\bar{\omega}$:

Step k: For each $L \in \omega_k$ which is not a singleton, find $i_0 := i(L) \in \tilde{L} := L \setminus \{\max\{i: i \in L\}\}$ such that $a_{i_0} = \min\{a_j: j \in \tilde{L}\}$ and $b_{i_0} = \min\{b_j: j \in \tilde{L}\}$. Put $L^- = \{i \in L: i \leq i_0\}$ and $L^+ = \{i \in L: i > i_0\}$, and define $\omega_{k+1} = \{L^-, L^+: L \in \omega_k \text{ is not singleton}\} \cup \{L \in \omega_k: L \text{ is a singleton}\}$.

The total dyadic filtration $\mathcal{F} = (\omega_0 \prec^d \dots \prec^d \omega_r)$ constructed by the algorithm is said to be *associated* to the NBF.

We point out that in Definition 2.8 in [8], the NBF matrices are defined by induction on the dimension of the matrix. It is easy to show that this definition is equivalent to ours. Observe that, up to permutation, an ultrametric matrix is an NBF matrix with $a_i = b_i$ (see [4]). Furthermore, if we also impose that $a_1 < \dots < a_{n-1} < a_n$ and $U_{ii} = a_i, i = 1, \dots, n$, one obtains the type-D matrices considered in [7].

Remark 3.

- (a) An NBF matrix is a GU matrix. The tree (T, \mathcal{F}) associated to the total dyadic filtration \mathcal{F} supports the GU matrix. We notice that all the atoms in this filtration are intervals in I , or equivalently, all nodes $L \in T$ are intervals in I . Moreover, $\alpha_L = a_{i(L)}, \beta_L = b_{i(L)}$.
- (b) From Definition 2(c), one gets $U_{ij} = a_{i(L)}$ for $(i, j) \in L^- \times L^+$ and $U_{ij} = b_{i(L)}$ for $(i, j) \in L^+ \times L^-$.
- (c) If U is in NBF, the filtration \mathcal{F} is not necessarily unique. In fact, at some step k there could exist several $i(L)$ satisfying the condition, but it can be shown (by induction on n) that the algorithm stops at $\bar{\omega}$ independently on the choice of $i(L)$. We describe all the filtrations associated to an NBF in Theorem 5(b).

To describe the permutations preserving the NBF of a matrix U , we use its GU property and the tree (T, \mathcal{F}) supporting it. Recall the total order $\leq_{\mathcal{F}}$ introduced in (2) also orders the disjoint $\leq_{\mathcal{F}}$ -intervals.

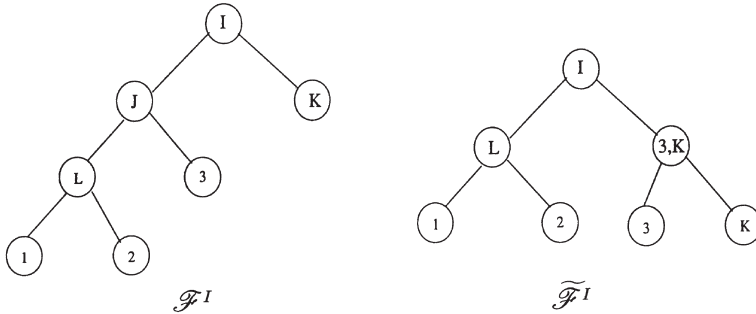


Fig. 2.

Take $L \in T$. We will fix a partition ω^L of L (formed by elements of T). If L is a leaf, we put $\omega^L = \{L\}$. When L is not a leaf, we define

$$J \in \omega^L \Leftrightarrow J \succ L, (\alpha_{p(J)}, \beta_{p(J)}) = (\alpha_L, \beta_L) \text{ and } [J \text{ is a leaf or } (\alpha_J, \beta_J) \neq (\alpha_L, \beta_L)].$$

Observe that the set $T^L = \{J \geq L : (\alpha_J, \beta_J) = (\alpha_L, \beta_L)\} \cup \omega^L$ is a dyadic tree, when endowed with the relation inherited from (T, \mathcal{F}) . The tree T^L has the tree root L and set of leaves ω^L . We denote by \mathcal{F}^L the filtration associated to T^L .

A total dyadic filtration $\tilde{\mathcal{F}}^L = (\tilde{\omega}_0 \prec^d \dots \prec^d \tilde{\omega}_r)$ of L is said to be ω^L -compatible if $\tilde{\omega}_0 = \{L\}$, $\tilde{\omega}_r = \omega^L$ and the atoms of every $\tilde{\omega}_k$ are the union of consecutive atoms of ω^L (consecutive with respect to the order $\leq_{\mathcal{F}}$ in intervals, in particular, they are $\leq_{\mathcal{F}}$ -intervals). By definition, \mathcal{F}^L is ω^L -compatible.

A permutation $\varphi_L : L \rightarrow L$ is said to be a ω^L -interval exchange if for every $J \in \omega^L$, $\varphi_L(J)$ is a $\leq_{\mathcal{F}}$ -interval of L and $\varphi_L : J \rightarrow \varphi_L(J)$ is increasing with respect to $\leq_{\mathcal{F}}$, i.e. $\varphi_L(i) \leq_{\mathcal{F}} \varphi_L(j)$ if $i \leq_{\mathcal{F}} j$, $i, j \in J$. We will also denote by φ_L the extension of this permutation to I , where we put $\varphi_L(i) = i$ if $i \notin L$.

In Fig. 2 we display \mathcal{F}^I for Example 1, as well as a $\tilde{\mathcal{F}}^I$ filtration which is ω^I -compatible. Observe that $\omega^I = \{\{1\}, \{2\}, \{3\}, K\}$.

Theorem 5. Let $I = \{1, \dots, n\}$ and the matrix U be in NBF. Then:

- (a) $\varphi : I \rightarrow I$ is a permutation such that $U^\varphi := (U_{\varphi^{-1}(i)\varphi^{-1}(j)} : i, j \in I)$ is in NBF if and only if φ is a composition of permutations φ_L , where φ_L is a ω^L -interval exchange and L satisfies $\alpha_L = \beta_L$.
- (b) Let \mathcal{F} be a fixed total dyadic filtration associated to the NBF. Then, the class of total dyadic filtrations associated to the NBF is constructed by making all possible replacements of \mathcal{F}^L by ω^L -compatible filtrations $\tilde{\mathcal{F}}^L$ of L for $L \in T$.

The proof is direct. Notice that in statements (a) and (b) of the theorem it suffices to restrict our attention to $L = I$ and those L satisfying $(\alpha_{\mathbf{p}(L)}, \beta_{\mathbf{p}(L)}) \neq (\alpha_L, \beta_L)$, because they generate dyadic maximal subtrees T^L .

For instance, in Example 1, the set of permutations which preserve the NBF are those which fix the points $\{1, 2, 3\}$.

7. Probabilistic insight and general results for potential matrices

Let U be a nonsingular matrix with U^{-1} a row DDM matrix. Let $\eta \geq \eta(U)$ and consider the sub-Markov kernel $P = \mathbb{1} - \eta^{-1}U^{-1}$. The properties of matrix U , from a probabilistic point of view, come from the fact that U is proportional to the potential of P given by $V := (\mathbb{1} - P)^{-1}$. By adding an absorbing state $\partial \notin I$, we can construct a Markov chain (X_m) with kernel \tilde{P} satisfying $\tilde{P}|_{I \times I} = P$. We refer to [1] for general considerations on Markov chains. Denote by \mathbb{P}_i the law of the chain starting from i and by \mathbb{E}_i the associated mean expected value operator. From the definition of V , we get that $V_{ij} = \mathbb{E}_i(\sum_{m \geq 0} 1_{\{X_m=j\}})$ is the expected number of visits to j starting from i . From the strong Markov property, one obtains $V_{ij} = \mathbb{P}_i\{T_{\{j\}} < \infty\}V_{jj}$, where in general T_J is the hitting time of a set $J \subseteq I$, that is the first (random) time that the chain visits J .

Thus, the ratio $V_{ij}/V_{jj} = U_{ij}/U_{jj}$ represents the probability that the chain starting from i ever visits j . This probability is one if and only if every path starting from i visits j before absorption, from which one deduces, for example, Theorem 3.2 in [8]. Moreover, in this general framework, for every exiting root r we can characterize the set $\mathcal{H}_r = \{j \in I: U_{jr} = U_{rr}\}$ as follows:

$$j \in \mathcal{H}_r \Leftrightarrow \mathbb{P}_j\{T_{\{r\}} < \infty\} = 1.$$

Hence, if there is only one root r , then the right-hand side of the above equivalence is true for all $j \in I$ and therefore, $\mathcal{H}_r = I$.

If $\mathbb{1} - P$ is a strictly row DDM matrix (all the row sums are strictly positive), then every vertex $i \in I$ is an exiting root and therefore, $\mathbb{P}_i\{T_{\{j\}} < \infty\} < 1$. This implies the necessary condition stated in [6]:

$$V_{jj} > \max\{V_{ij}: i \in I \setminus \{j\}\}.$$

Also, the implication $U_{ij} = 0 \Rightarrow (U^{-1})_{ij} = 0$ for $i \neq j$ (see the additional property in Theorem 3.6 in [11]) has a simple meaning because it is equivalent to $\mathbb{P}_i\{T_{\{j\}} < \infty\} = 0 \Rightarrow P_{ij} = 0$, which is trivial.

The terms $\eta \sum_{j \in I} U_{ij}$ involved in the determination of exiting roots can be described in probabilistic terms. In fact if the chain starts from I , the time of absorption is $T_\partial := \inf\{m: X_m = \partial\} = \sum_{m \geq 0} 1_{\{X_m \in I\}}$. Then for $i \in I$

$$\mathbb{E}_i(T_\partial) = \sum_{m \geq 0} \sum_{j \in I} P_{ij}^{(m)} = \eta \sum_{j \in I} U_{ij}.$$

Intuitively, the site minimizing this quantity should be an exiting root, as it was proven in Theorem 1.

In the next result, we get an extra property on the structure of the sets $\{\mathcal{H}_r : r \in \mathcal{R}\}$ by using probabilistic tools.

Proposition 2. *Let U be the inverse of a row DDM matrix. Let $r \in \mathcal{R}$, $j \in \mathcal{H}_r$, $k \notin \mathcal{H}_r$. Then*

$$\mathbb{P}_j\{T_{\{k\}} < T_{\{r\}}\} = 0 \quad \text{and} \quad U_{jk} = U_{rk}.$$

Proof. Since $k \notin \mathcal{H}_r$ and $j \in \mathcal{H}_r$, we have $\mathbb{P}_k\{T_{\{r\}} = \infty\} > 0$ and $\mathbb{P}_j\{T_{\{r\}} < \infty\} = 1$. Hence, the following inequality

$$0 = \mathbb{P}_j\{T_{\{r\}} = \infty\} \geq \mathbb{P}_j\{T_{\{k\}} < T_{\{r\}}\} \mathbb{P}_k\{T_{\{r\}} = \infty\}$$

implies $\mathbb{P}_j\{T_{\{k\}} < T_{\{r\}}\} = 0$.

The second relation follows by the strong Markov property, conditioning on the first visit from j to r or k . In fact,

$$U_{jk} = \mathbb{P}_j\{T_{\{k\}} < T_{\{r\}}\}U_{kk} + \mathbb{P}_j\{T_{\{r\}} < T_{\{k\}}\}U_{rk} = U_{rk},$$

where the last equality follows from the above discussion. \square

Schur’s decomposition has also a probabilistic meaning. Assume that $J \subseteq I$, and we would like to study the Markov chain (Y_m) induced on J , whose transition matrix Q is given by

$$\begin{aligned} Q_{ij} &:= \mathbb{P}_i\{T_J < \infty, X_{T_J} = j\} \\ &= P_{ij} + \mathbb{P}_i\{1 < T_J < \infty, X_{T_J} = j\} \quad \text{for } i, j \in J. \end{aligned}$$

Since the potential of this new chain in J is the same as for the initial chain, as the expected number of visits is the same, we obtain that $\mathbb{1} - Q = (V_{J \times J})^{-1}$, but from Schur’s decomposition

$$(V_{J \times J})^{-1} = (\mathbb{1} - P)_{J \times J} - (\mathbb{1} - P)_{J \times K} ((\mathbb{1} - P)_{K \times K})^{-1} (\mathbb{1} - P)_{K \times J}.$$

In particular, $i \in J$ is an exiting root for Q (or equivalently for the chain (Y_m)) if and only if i is an exiting root for P or if there is a path from i to the absorbing state $\hat{0}$ passing only through K . This statement is what appears in Lemma 3.1(ii) in [8]. We point out that our results in Lemmas 6 and 7 are a sort of reciprocal of the formula stated in the proof of Lemma 3.1(iii) in [8].

So far we have discussed how row DDM matrices arise in probability theory. In the sequel, we shall assume that U is the inverse of a nonsingular M-matrix $a\mathbb{1} - P$, that is we assume that a is strictly larger than $\rho := \rho(P)$, the spectral radius of the nonnegative matrix P . In general P is not sub-Markovian except in the row DD case. Nevertheless, U has a probabilistic interpretation as an h -transform of a suitable potential. In order to explain the main ideas here, we assume that P is irreducible.

Therefore, by the Perron–Frobenius theorem there exists a unique strictly positive right eigenvector h : $Ph = \rho h$. Consider the Markov kernel R given by

$$R_{ij} = \rho^{-1} \frac{h_j}{h_i} P_{ij}.$$

A direct computation shows that

$$P_{ij}^{(n)} = \rho^n \frac{h_i}{h_j} R_{ij}^{(n)} \quad \text{for } n \geq 0.$$

Therefore, we get

$$U_{ij} = a^{-1} \sum_{n=0}^{\infty} a^{-n} P_{ij}^{(n)} = a^{-1} \frac{h_i}{h_j} \sum_{n=0}^{\infty} \left(\frac{\rho}{a}\right)^n R_{ij}^{(n)}.$$

Define W the potential

$$W = \sum_{n=0}^{\infty} \left(\frac{\rho}{a}\right)^n R^n,$$

associated to the sub-Markovian kernel $\rho/a R$. Then, we have

$$U_{ij} = a^{-1} \frac{h_i}{h_j} W_{ij},$$

and U is an h -transform of W . This result allows us to give a probabilistic insight into Theorem 3.9 in [8]. We use definitions and notations introduced therein. The condition “ j does not have access to k in $G_i(P)$ ” is the same as “ j does not have access to k in $G_i(R)$ ” because the connections are the same under P or R . In probabilistic terms, this condition is stated as $\mathbb{P}_j\{T_{\{k\}} < T_{\{i\}}\} = 0$, where \mathbb{P} is the law of the underline chain defined by the kernel $\rho/a R$ (adding of course an absorbing state). Under this hypothesis, the strong Markov property implies

$$\begin{aligned} W_{jk} &= \mathbb{P}_j\{T_{\{k\}} < \infty\} W_{kk} = \mathbb{P}_j\{T_{\{i\}} < T_{\{k\}} < \infty\} W_{kk} \\ &= \mathbb{P}_j\{T_{\{i\}} < \infty\} \mathbb{P}_i\{T_{\{k\}} < \infty\} W_{kk} = W_{ji} W_{ik} / W_{ii}. \end{aligned} \quad (17)$$

Using the relation between U and W , one gets the same formula for U . This proves the first part of Theorem 3.9 in [8]. The second part of this theorem follows in a similar way, by noticing that the second equality in (17) becomes a strict inequality $>$, whenever “ j has access to k in $G_i(P)$ ”.

7.1. Final comment

For U , the inverse of a row DDM matrix, we provide an estimation of $\eta(U) = \max\{(U^{-1})_{ii} : i \in I\}$ in terms of U . Consider $\epsilon(U) := \min\{U_{ii} - \max\{U_{ji} : j \neq i\} : i \in I\}$. Then $\eta(U) \leq \epsilon(U)^{-1}$. In fact, from the row DDM property we get

$$(U^{-1})_{ii} U_{ii} = 1 - \sum_{j \neq i} (U^{-1})_{ij} U_{ji} \leq 1 - (U_{ii} - \epsilon(U)) \sum_{j \neq i} (U^{-1})_{ij}$$

$$\leq 1 + (U_{ii} - \epsilon(U))(U^{-1})_{ii},$$

from which $(U^{-1})_{ii} \leq \epsilon(U)^{-1}$ and the claim follows.

Notice that $\epsilon(U) \geq 1$ implies $\eta(U) \leq 1$, and then $P = \mathbb{I} - U^{-1}$ is a sub-Markovian kernel. If in addition, U is a GU matrix, we get that $\mathbb{I} - U^{-1}$ is a double sub-Markovian kernel and this is also the case for all the levels L in the tree, because $\eta(U_L) \leq \eta(U)$ (see (3)).

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