

Research Article

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On monotone Markov chains and properties of monotone matrix roots

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Abstract: Monotone matrices are stochastic matrices that satisfy the monotonicity conditions as introduced by Daley in 1968. Monotone Markov chains are useful in modeling phenomena in several areas. Most previous work examines the embedding problem for Markov chains within the entire set of stochastic transition matrices, and only a few studies focus on the embeddability within a specific subset of stochastic matrices. This article examines the embedding in a discrete-time monotone Markov chain, i.e., the existence of monotone matrix roots. Monotone matrix roots of (2×2) monotone matrices are investigated in previous work. For (3×3) monotone matrices, this article proves properties that are useful in studying the existence of monotone roots. Furthermore, we demonstrate that all (3×3) monotone matrices with positive eigenvalues have an m th root that satisfies the monotonicity conditions (for all values $m \in \mathbb{N}$, $m \geq 2$). For monotone matrices of order $n > 3$, diverse scenarios regarding the matrix roots are pointed out, and interesting properties are discussed for block diagonal and diagonalizable monotone matrices.

Keywords: monotone Markov chain, monotone matrix, matrix roots, embedding problem

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1 Introduction

The embedding problem as introduced by Elfving in [1] investigates whether or not a discrete-time Markov chain is embeddable in a continuous-time Markov chain [2,3]. A Markov chain with a transition matrix P is continuous embeddable in case there exists a Markov generator G such that $e^G = P$. Besides continuous embeddability, discrete embeddability is being studied. It regards the problem of whether or not a discrete-time Markov chain can be embedded in a discrete-time Markov chain [4,5]. Particularly, the discrete embedding problem involves the question of whether, for a given Markov chain regarding time unit 1, there exists a compatible Markov chain regarding time unit $\frac{1}{m}$ ($m \in \mathbb{N}$, $m \geq 2$). The transition matrix of a Markov chain enables us to reformulate this problem: A Markov chain with a transition matrix P is discrete embeddable in case there exist a stochastic matrix A and a number $m \in \mathbb{N}$, $m \geq 2$ satisfying $P = A^m$. Such a matrix A is in fact an m th root of P within the set of stochastic matrices and is called a stochastic m th root of P . Several methods exist for computing matrix roots without focusing on stochastic roots [6,7]. Stochastic roots of $(n \times n)$ transition matrices are examined in some recent work [8,9], including studies that address in particular $n = 2$ and $n = 3$ [10,11]. In case for a transition matrix P there exists a stochastic root, we say that the matrix P is discrete embeddable within the set of stochastic matrices.

In building a Markov model, there are different possible situations in which one has to deal with a lack of data. One of these situations occurs when data are only available regarding time intervals that are greater

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than the time unit of the Markov model. In such a situation, the stochastic m th roots nevertheless provide insight into the transition probabilities regarding time intervals with length $\frac{1}{m}$ ($m \in \mathbb{N}$, $m \geq 2$). In this way, a stochastic m th root enables us to find parameter estimations for a Markov chain in case there is a lack of appropriate data.

In modeling a specific context, the transition matrix P of the Markov chain satisfies specific conditions. In examining the embeddability in such a situation, the existence of an arbitrary stochastic root is not satisfactory since the same specific conditions have to be fulfilled by the stochastic root of P . In this way, the transition matrix P as well as its matrix roots are both elements of the same specific subset of stochastic matrices. Recently, several articles have investigated matrix roots and the embedding problem within a specific subset of stochastic matrices: Matrix roots are examined within the set of symmetric and monomial matrices [12], within the set of circulant matrices [13], and within the set of state-wise monotone matrices [14]. The embedding problem for reversible Markov chains is investigated in [15] and for Kimura Markov matrices in [16].

Monotone Markov chains are introduced by Daley in [17] and further investigated by Keilson and Kester in [18]. Several authors point out the importance of monotone Markov models in practice for diverse contexts: for example, monotone Markov models for intergenerational occupational mobility, where the states are occupational categories that have a natural ranking from worst to best, and the transition probability p_{ij} expresses the probability that a parent in state i will have a child in state j [19]. As well as monotone Markov models where the states are income classes arranged in an increasing order can be useful in modeling intergenerational income mobility [20]. Tests for stochastic monotonicity in intergenerational mobility tables are introduced in [21]. Monotone matrices also play an important role in equal-input modeling [22].

Monotone Markov models are useful in examining the evolution of credit ratings based on a credit rating transition matrix where the states are the ranked possible credit classes, with the first state being the highest rating *AAA*. A credit rating transition matrix should satisfy the monotonicity conditions [23]. The rating transition matrix is typically estimated for a 1-year period. One of the reasons for this is that the number of transitions within a shorter period is too small to result in a valid estimation for the transition probabilities [24]. In [24], the embedding problem in a continuous Markov chain for a credit rating transition matrix is examined. A square root of a yearly credit rating transition matrix would provide insights regarding the probability of the transition from rating i to rating j on semi-annual base. This example illustrates that m th roots of a monotone transition matrix provide useful insights. In case for a monotone transition matrix P there exists a monotone root, we say that the matrix P is discrete embeddable within the set of monotone matrices.

In this article, properties of the set of monotone matrices are examined. Furthermore, matrix roots and the discrete embedding problem are studied within this set. The article is organized as follows: Section 2 recalls some definitions and properties of the set of monotone matrices. In Section 3, matrix roots and the discrete embedding problem are discussed for $n = 2$. Section 4 examines the monotonicity conditions for roots of (3×3) monotone matrices. Section 5 discusses generalizations for $n > 3$. The article concludes with avenues for future research in Section 6.

2 The set of monotone matrices

A transition matrix of a Markov chain with n states is a stochastic matrix of order $(n \times n)$. Let us introduce the set \mathcal{S}_n of stochastic $(n \times n)$ matrices:

$$\mathcal{S}_n = \left\{ M = (m_{ij}) \in \mathbb{R}^{n \times n} \left| \sum_{j=1}^n m_{ij} = 1 \quad \text{and} \quad m_{ij} \geq 0 \quad \forall i, j \in \{1, \dots, n\} \right. \right\}.$$

The concept of monotone matrix is introduced by Daley [17]. A monotone matrix is a stochastic matrix satisfying the following monotonicity conditions:

$$\sum_{j=r}^n m_{lj} \geq \sum_{j=r}^n m_{kj} \quad \forall l > k, \quad \forall r \in \{1, \dots, n\}. \quad (1)$$

The set of $(n \times n)$ monotone matrices can therefore be described as

$$\mathbb{M}_n = \mathcal{S}_n \cap \text{MC}_n,$$

where MC_n is the set of $(n \times n)$ matrices defined as follows:

$$\text{MC}_n = \left\{ M = (m_{ij}) \in \mathbb{R}^{n \times n} \left| \sum_{j=r}^n m_{lj} \geq \sum_{j=r}^n m_{kj} \quad \forall l > k, \quad \forall r \in \{1, \dots, n\} \right. \right\}.$$

A monotone transition matrix is characterized by the fact that each row l stochastically dominates each higher row k . Since, for a matrix M with all row sums equal (to 1), $r = 1$ results in redundant conditions, and because of transitivity, monotonicity for $M \in \mathcal{S}_n$ can be expressed by the following $(n - 1)^2$ conditions:

$$M \in \text{MC}_n \quad \Leftrightarrow \quad \sum_{j=r}^n m_{k+1,j} - \sum_{j=r}^n m_{kj} \geq 0 \quad \forall k \in \{1, \dots, n - 1\}, \quad \forall r \in \{2, \dots, n\}. \quad (2)$$

With regard to the eigenvalues of a monotone matrix, there are already some characteristics known: A monotone matrix is a stochastic matrix and has therefore always 1 as trivial eigenvalue. By introducing for $M \in \mathcal{S}_n$, the dominance matrix $D(M)$ as the $((n - 1) \times (n - 1))$ matrix with (k, l) th element equal to $\sum_{j=1}^l m_{kj} - \sum_{j=1}^l m_{k+1,j}$, Conlisk defined monotonicity for $M \in \mathcal{S}_n$ as follows: $M \in \mathbb{M}_n \Leftrightarrow D(M) \geq 0$ and concluded that for a monotone matrix $M \in \mathbb{M}_n$, the nontrivial eigenvalue with largest modulus is always nonnegative [19].

With regard to the trace $\text{tr}(M)$, one can remark for $M \in \mathcal{S}_n$ that $0 \leq \text{tr}(M) \leq n$. The subset $\mathbb{M}_n \subset \mathcal{S}_n$ of monotone matrices is further characterized as follows:

$$\text{tr}(M) \geq 1 \quad \forall M \in \mathbb{M}_n. \quad (3)$$

This insight follows from using iteratively the monotonicity conditions (1):

$$1 = \sum_{j=1}^n m_{1j} \leq m_{11} + \sum_{j=2}^n m_{2j} \leq m_{11} + m_{22} + \sum_{j=3}^n m_{3j} \leq \dots \leq m_{11} + m_{22} + \dots + m_{nn} = \text{tr}(M).$$

It is well known that for $M \in \mathbb{M}_n$, all powers are monotone ([18], Theorem 1.2). In this way, the matrix power preserves the monotonicity conditions. The aim is now to investigate whether there exist matrix roots of $M \in \mathbb{M}_n$ that still satisfy the monotonicity conditions (1).

A monotone Markov chain with transition matrix $P \in \mathbb{M}_n$ is discrete embeddable within the set \mathbb{M}_n in case there exists a value $m \in \mathbb{N}$, $m \geq 2$, and a monotone matrix $A \in \mathbb{M}_n$ such that $P = A^m$. The monotone Markov chain is said to be continuous embeddable within the set \mathbb{M}_n in case there exists a compatible continuous monotone Markov chain with generator G such that $P = e^G$. Such a generator $G = (g_{ij})$ satisfies $g_{ij} \geq 0 \quad \forall i \neq j$ and $g_{ii} = -\sum_{j \neq i} g_{ij}$ and $e^{tG} \in \mathbb{M}_n \quad \forall t \geq 0$. There is an efficient way to verify the monotonicity conditions for the continuous Markov chain ([18], Theorem 2.1):

$$e^{tG} \in \mathbb{M}_n \quad \forall t \geq 0 \quad \Leftrightarrow \quad \sum_{j=r}^n g_{k+1,j} - \sum_{j=r}^n g_{kj} \geq 0 \quad \forall k \in \{1, \dots, n - 1\}, \quad \forall r \neq k + 1. \quad (4)$$

A Markov generator satisfying equation (4) is called a monotone generator. In some situations, the problem of matrix roots of P can be examined via the Markov generator G since $e^{G/m}$ is an m th root of P .

Stochastic matrix roots and the general discrete embedding problem that examines the existence of m th roots of the transition matrix within the set \mathcal{S}_n have been studied in previous work. Therefore, this article focuses on the question of whether for $M \in \mathbb{M}_n = \mathcal{S}_n \cap \text{MC}_n$, the monotonicity conditions are still satisfied

for a matrix root of M . In the following sections, specific properties regarding matrix roots are examined more in detail for the particular cases of two-state and three-state monotone Markov chains.

3 Roots of (2×2) monotone matrices

A matrix $P = (p_{ij}) \in \mathbb{M}_2$ has eigenvalues 1 and $\lambda \geq 0$ according to equation (3). The case $\lambda = 0$ corresponds to an idempotent matrix P that has itself as m th root. The case $\lambda > 0$ gives rise to a continuous embeddable matrix P ([2], Proposition 2) with unique Markov generator $G = \frac{\log(\text{tr}(P) - 1)}{\text{tr}(P) - 2} \begin{pmatrix} -p_{12} & p_{12} \\ p_{21} & -p_{21} \end{pmatrix}$ [4]. The corresponding matrix roots $\sqrt[m]{P} = e^{G/m}$ are monotone since G is a monotone generator (according to equation (4)) and can be expressed as follows [10,25]:

$$\sqrt[m]{P} = \frac{1}{p_{12} + p_{21}} \begin{pmatrix} p_{21} + p_{12} \sqrt[m]{\lambda} & p_{12} - p_{12} \sqrt[m]{\lambda} \\ p_{21} - p_{21} \sqrt[m]{\lambda} & p_{12} + p_{21} \sqrt[m]{\lambda} \end{pmatrix}. \quad (5)$$

These insights brings us, in accordance with the result in [22], to the formulation of Theorem 1.

Theorem 1. *Each monotone matrix P of order (2×2) has $\sqrt[m]{P}$ (as defined in equation (5)) as monotone m th root (for all $m \in \mathbb{N}$, $m \geq 2$). Each monotone Markov chain with two states is discrete embeddable and continuous embeddable within the set of monotone matrices.*

One can verify that the monotone m th root $\sqrt[m]{P}$, as introduced in equation (5), equals $\sqrt[m]{P} = T \times \sqrt[m]{D} \times T^{-1}$, where $D = \text{diag}(1, \lambda)$ is the diagonal matrix with the eigenvalues 1 and λ as diagonal elements. The matrix T is a transformation matrix with columns that are right eigenvectors of P . Hence, $P = T \times D \times T^{-1}$ and $\sqrt[m]{D} = \text{diag}(1, \sqrt[m]{\lambda})$.

The result that $\sqrt[m]{P} \in \mathbb{M}_2$, for $P \in \mathbb{M}_2$, is the motivation to examine properties of the matrix roots $\sqrt[m]{P} = T \times \sqrt[m]{D} \times T^{-1}$ for diagonalizable matrices P of order $n > 2$ to find out whether or not Theorem 1 can be generalized.

4 Roots and embedding conditions for (3×3) monotone matrices

The following theorem provides specific properties of the eigenvalues $\lambda_1 = 1$, λ_2 and λ_3 of a matrix $P \in \mathbb{M}_3$ as well as necessary embedding conditions.

Theorem 2. *For a monotone matrix P of order (3×3) holds the following:*

The eigenvalues 1, λ_2 , and λ_3 of P are real-valued. If $\lambda_2 \geq \lambda_3$, then $\lambda_2 \geq 0$ and $\lambda_3 \geq -\lambda_2$. In case the matrix P is discrete embeddable within \mathcal{S}_3 holds $\lambda_2 \geq 0$ and $\lambda_3 \geq \max\{-\lambda_2, -0.5\}$. Furthermore, in case P is discrete embeddable within \mathbb{M}_3 with an m th root for $m \geq 2$ even number, both λ_2 and λ_3 are nonnegative.

Proof. Assume $|\lambda_2| \geq |\lambda_3|$. Then, according to [19], λ_2 is nonnegative. Consequently, the characteristic equation of P has $\lambda_1 = 1$ and λ_2 as real-valued solutions and, therefore, also $\lambda_3 \in \mathbb{R}$. Furthermore, according to equation (3) holds that $\text{tr}(P) = 1 + \lambda_2 + \lambda_3 \geq 1$. Hence, $\lambda_2 \geq 0$ and $\lambda_3 \geq -\lambda_2$.

In case the monotone matrix P is discrete embeddable within \mathcal{S}_3 , its eigenvalues are elements of $\Theta_3 = \{(x, y) \in \mathbb{R}^2 | x \geq -0.5; x - 1 \leq \sqrt{3}y \leq 1 - x\}$ [26] and therefore, additionally, $\lambda_3 \geq -0.5$.

In case P is discrete embeddable within \mathbb{M}_3 , there exists a monotone matrix $A \in \mathbb{M}_3$ such that $P = A^m$. Denoting the eigenvalues of A as $\mu_1 = 1$, μ_2 and μ_3 , the eigenvalues of $P = A^m$ are equal to 1, $(\mu_2)^m$ and $(\mu_3)^m$. Since $\mu_2 \in \mathbb{R}$, and $\mu_3 \in \mathbb{R}$, for m even number holds that $(\mu_2)^m \geq 0$ and $(\mu_3)^m \geq 0$. \square

The eigenvalues $\lambda_1 = 1$ and $\lambda_2 \geq \lambda_3$ of the monotone matrix P satisfy $\lambda_2 \geq 0$. In case λ_3 is negative, the discussion of m th roots is, in accordance to Theorem 2, restricted to m odd. In other words, m th roots are examined for $m \in \mathbb{N}(\lambda_3)$:

$$\begin{aligned}\mathbb{N}(\lambda_3) &= \mathbb{N} \setminus \{0\} && \text{in case } \lambda_3 \geq 0 \\ &= \{m \in \mathbb{N} \setminus \{0\} \mid m \text{ odd}\} && \text{in case } \lambda_3 < 0.\end{aligned}$$

A matrix P of \mathbb{M}_3 is a stochastic matrix with real-valued eigenvalues. Roots of (3×3) stochastic matrices with real eigenvalues are studied in detail in [11], and those findings are therefore useful in what follows. The aim is now to investigate whether there exist matrix roots of $P \in \mathbb{M}_3$ that satisfy the monotonicity conditions. For $M \in \mathcal{S}_3$, the conditions in equation (1) can be reformulated as follows:

$$M = (m_{ij}) \in \mathbb{M}_3 \Leftrightarrow \begin{cases} m_{33} \geq m_{23} \geq m_{13} \\ m_{31} \leq m_{21} \leq m_{11} \end{cases}. \quad (6)$$

For a (3×3) monotone matrix, a positive spectrum is a necessary condition for the existence of a monotone Markov generator. For $P \in \mathbb{M}_3$ with positive eigenvalues and minimal polynomial of degree ≤ 2 , a unique monotone generator G is guaranteed ([22], Prop. 4.3). The matrix $P = e^G$ is then discrete embeddable within the set of monotone matrices and Theorem 3 follows.

Theorem 3. *Each monotone matrix P of order (3×3) with positive eigenvalues and minimal polynomial of degree ≤ 2 , has for each $m \in \mathbb{N}$, $m \geq 2$, the m th root $\sqrt[m]{P} = e^{G/m}$ within the set \mathbb{M}_3 , where G is the unique monotone Markov generator of P .*

Matrices $P \in \mathbb{M}_3$ with positive eigenvalues and minimal polynomial of degree ≤ 2 are diagonalizable. For these, and for all diagonalizable monotone matrix P more in general, the monotonicity properties of matrix roots are further examined in the following section.

4.1 Diagonalizable monotone matrices of order 3

For a diagonalizable matrix $P \in \mathbb{M}_3$, there exists a transformation matrix T so that $T^{-1} \times P \times T = D$ with $D = \text{diag}(1, \lambda_2, \lambda_3)$ the diagonal matrix with diagonal elements 1, λ_2 and λ_3 . Let us denote, for all $m \in \mathbb{N}(\lambda_3)$, $\sqrt[m]{D} = \text{diag}(1, \sqrt[m]{\lambda_2}, \sqrt[m]{\lambda_3})$ and $\sqrt[m]{P} = T \times \sqrt[m]{D} \times T^{-1}$. The matrix $\sqrt[m]{P}$ is an m th root of P and has all row sums equal to 1 [11].

Expressing the diagonalizable matrices P and $\sqrt[m]{P}$ by their projections P_1, P_2 and P_3 results in the spectral decompositions:

$$P = P_1 + \lambda_2 P_2 + \lambda_3 P_3 \quad \text{and} \quad \sqrt[m]{P} = P_1 + \sqrt[m]{\lambda_2} P_2 + \sqrt[m]{\lambda_3} P_3.$$

Since both P and its m th root $\sqrt[m]{P}$ have the same projections, it has some advantages to reformulate the monotonicity conditions (6) based on the projections as in Lemma 4. The notation δ refers to Kronecker delta.

Lemma 4. *For $A = (a_{ij}) \in \mathcal{S}_3$ with eigenvalues $1 = \mu_1 \geq \mu_2 \geq \mu_3$ and A_2 the projection corresponding to μ_2 holds*

$$\begin{aligned}a_{il} \geq a_{jl} &\Leftrightarrow (A_2)_{il} - (A_2)_{jl} \geq \frac{\mu_3}{\mu_2 - \mu_3}(\delta_{jl} - \delta_{il}) \text{ in case } \mu_2 \neq \mu_3 \\ a_{il} \geq a_{jl} &\Leftrightarrow \mu_3(\delta_{jl} - \delta_{il}) \leq 0 \quad \text{in case } \mu_2 = \mu_3.\end{aligned}$$

Proof. Since the projections satisfy $A_1 + A_2 + A_3 = I_3$, where $I_3 = (\delta_{il})$ is the identity matrix of order 3, the spectral decomposition of $A = A_1 + \mu_2 A_2 + \mu_3 A_3$ can be rewritten as $A = (1 - \mu_3)A_1 + (\mu_2 - \mu_3)A_2 + \mu_3 I_3$. Moreover, the projection A_1 has all its rows equal and therefore:

$$a_{il} \geq a_{jl} \Leftrightarrow (\mu_2 - \mu_3)[(A_2)_{il} - (A_2)_{jl}] \geq \mu_3(\delta_{jl} - \delta_{il}). \quad (7)$$

That is, in case $\mu_2 > \mu_3$, equivalent with $(A_2)_{il} - (A_2)_{jl} \geq \frac{\mu_3}{\mu_2 - \mu_3}(\delta_{jl} - \delta_{il})$.

In case $\mu_2 = \mu_3$, equation (7) results in: $a_{il} \geq a_{jl} \Leftrightarrow \mu_3(\delta_{jl} - \delta_{il}) \leq 0$. \square

In what follows, the monotonicity of the matrix root $\sqrt[m]{P}$ is examined for alternative possible scenarios for the eigenvalues λ_2 and λ_3 .

Lemma 5. *For a monotone matrix $P = P_1 + \lambda_2 P_2 + \lambda_3 P_3$ with eigenvalues $1 = \lambda_1 \geq \lambda_2 > \lambda_3$ and $m \in \mathbb{N}(\lambda_3)$ holds that the m th root $\sqrt[m]{P} = P_1 + \sqrt[m]{\lambda_2} P_2 + \sqrt[m]{\lambda_3} P_3$ satisfies the monotonicity conditions if and only if*

$$\min\{(P_2)_{33} - (P_2)_{23}, (P_2)_{11} - (P_2)_{21}\} \geq \frac{\sqrt[m]{\lambda_3}}{\sqrt[m]{\lambda_3} - \sqrt[m]{\lambda_2}}.$$

Proof. According to Lemma 4, for $P = P_1 + \lambda_2 P_2 + \lambda_3 P_3$, the monotonicity conditions (6) are equivalent with

$$\begin{aligned} (P_2)_{33} - (P_2)_{23} &\geq \frac{\lambda_3}{\lambda_3 - \lambda_2}, \quad (P_2)_{23} - (P_2)_{13} \geq 0, \\ (P_2)_{11} - (P_2)_{21} &\geq \frac{\lambda_3}{\lambda_3 - \lambda_2}, \quad (P_2)_{21} - (P_2)_{31} \geq 0. \end{aligned} \quad (8)$$

In a similar way, for $\sqrt[m]{P} = P_1 + \sqrt[m]{\lambda_2} P_2 + \sqrt[m]{\lambda_3} P_3$, the monotonicity conditions can be expressed as follows:

$$\begin{aligned} (P_2)_{33} - (P_2)_{23} &\geq \frac{\sqrt[m]{\lambda_3}}{\sqrt[m]{\lambda_3} - \sqrt[m]{\lambda_2}}, \quad (P_2)_{23} - (P_2)_{13} \geq 0, \\ (P_2)_{11} - (P_2)_{21} &\geq \frac{\sqrt[m]{\lambda_3}}{\sqrt[m]{\lambda_3} - \sqrt[m]{\lambda_2}}, \quad (P_2)_{21} - (P_2)_{31} \geq 0. \end{aligned} \quad (9)$$

Since P is a monotone matrix, and therefore equation (8) holds, equation (9) is fulfilled if and only if $(P_2)_{33} - (P_2)_{23} \geq \frac{\sqrt[m]{\lambda_3}}{\sqrt[m]{\lambda_3} - \sqrt[m]{\lambda_2}}$ and $(P_2)_{11} - (P_2)_{21} \geq \frac{\sqrt[m]{\lambda_3}}{\sqrt[m]{\lambda_3} - \sqrt[m]{\lambda_2}}$, which proves the theorem. \square

Theorem 6. *For a diagonalizable monotone matrix $P = P_1 + \lambda_2 P_2 + \lambda_3 P_3$ with nonnegative eigenvalues $\lambda_2 \geq \lambda_3 \geq 0$, the monotonicity conditions (6) also hold for the matrix root $\sqrt[m]{P} = P_1 + \sqrt[m]{\lambda_2} P_2 + \sqrt[m]{\lambda_3} P_3$, and this for all $m \in \mathbb{N} \setminus \{0\}$.*

Proof. The configurations $\lambda_2 = \lambda_3 = 1$, and $\lambda_2 = 1, \lambda_3 = 0$, and $\lambda_2 = \lambda_3 = 0$ correspond to an idempotent matrix P that has itself as matrix root. The configurations $\lambda_2 = 1 > \lambda_3 > 0$ and $1 > \lambda_2 = \lambda_3 > 0$ are already covered by Theorem 3.

In case $1 > \lambda_2 > \lambda_3 = 0$, the conditions formulated in Lemma 5 are identical for P and its m th root $\sqrt[m]{P}$. Hence, for a monotone matrix P also the root matrix $\sqrt[m]{P}$ satisfies the monotonicity conditions (6).

In case $1 > \lambda_2 > \lambda_3 > 0$, according to Lemma 5, the m th root $\sqrt[m]{P}$ satisfies the monotonicity conditions if and only if $\min\{(P_2)_{33} - (P_2)_{23}, (P_2)_{11} - (P_2)_{21}\} \geq \frac{\sqrt[m]{\lambda_3}}{\sqrt[m]{\lambda_3} - \sqrt[m]{\lambda_2}}$. Besides, since P is a monotone matrix, we know that $\min\{(P_2)_{33} - (P_2)_{23}, (P_2)_{11} - (P_2)_{21}\} \geq \frac{\lambda_3}{\lambda_3 - \lambda_2}$. By rewriting $\frac{\sqrt[m]{\lambda_3}}{\sqrt[m]{\lambda_3} - \sqrt[m]{\lambda_2}} = \frac{1}{1 - \frac{\sqrt[m]{\lambda_2}}{\sqrt[m]{\lambda_3}}}$ and observing that $1 < \sqrt[m]{\frac{\lambda_2}{\lambda_3}} < \frac{\lambda_2}{\lambda_3}$ for $\lambda_2 > \lambda_3 > 0$ holds $\min\{(P_2)_{33} - (P_2)_{23}, (P_2)_{11} - (P_2)_{21}\} \geq \frac{\lambda_3}{\lambda_3 - \lambda_2} > \frac{\sqrt[m]{\lambda_3}}{\sqrt[m]{\lambda_3} - \sqrt[m]{\lambda_2}}$. Hence, $\sqrt[m]{P}$ satisfies the monotonicity conditions. \square

Diagonalizable monotone matrices of order (3×3) with positive eigenvalues and degree of the minimal polynomial maximum equal to 2 are discrete embeddable within \mathbb{M}_3 (according to Theorem 3). More in general, Theorem 6 guarantees that a diagonalizable matrix $P \in \mathbb{M}_3$ with nonnegative eigenvalues is discrete embeddable within \mathbb{M}_3 in case at least one of the roots $\sqrt[m]{P}$ is a stochastic matrix. This insight results in the following corollary.

Corollary 6.1. *Each diagonalizable monotone matrix P of order (3×3) with nonnegative eigenvalues and for which $\sqrt[m]{P} \in \mathcal{S}_3$ (for some $m \in \mathbb{N}$, $m \geq 2$) is discrete embeddable within the set of monotone matrices.*

Theorem 7. *Let $P = P_1 + \lambda_2 P_2 + \lambda_3 P_3$ be a diagonalizable monotone matrix with eigenvalues $\lambda_2 \geq 0 > \lambda_3$. In case for n odd, the matrix root $\sqrt[n]{P} = P_1 + \sqrt[n]{\lambda_2} P_2 + \sqrt[n]{\lambda_3} P_3$ satisfies the monotonicity conditions (6). Then all matrix roots $\sqrt[m]{P} = P_1 + \sqrt[m]{\lambda_2} P_2 + \sqrt[m]{\lambda_3} P_3$ with $m < n$ odd value satisfy the monotonicity conditions (6).*

Proof. The eigenvalues of $P \in \mathbb{M}_3$ satisfy $\lambda_3 \geq -\lambda_2 \geq 0$ (according to Theorem 2). Hence, for P with $\lambda_2 \geq 0 > \lambda_3$ is $\frac{\sqrt[m]{\lambda_3}}{\sqrt[m]{\lambda_3} - \sqrt[m]{\lambda_2}} = \frac{1}{1 + \sqrt[m]{\frac{\lambda_2}{-\lambda_3}}}$ an increasing function of m , and the proof follows from Lemma 5. \square

For a diagonalizable monotone matrix P that has a negative eigenvalue, one can remark that in case the monotonicity properties (6) hold for the matrix root $\sqrt[m]{P}$ (with m a particular value in $\mathbb{N}(\lambda_3)$), this is automatically also the case for $\sqrt[3]{P}$ (as a result of Theorem 7). Therefore, if the third root $\sqrt[3]{P}$ does not satisfy the monotonicity conditions, this is necessary and sufficient to conclude that none of the roots $\sqrt[m]{P}$ (for all $m \in \mathbb{N}(\lambda_3)$) satisfies the monotonicity conditions.

For example, for the monotone matrix $P = \begin{pmatrix} 0.2 & 0.2 & 0.6 \\ 0.2 & 0.1 & 0.7 \\ 0.1 & 0.1 & 0.8 \end{pmatrix}$ with eigenvalues $\lambda_2 = \frac{1+\sqrt{5}}{20}$ and $\lambda_3 = \frac{1-\sqrt{5}}{20}$, the second projection equals $P_2 = \begin{pmatrix} 0.583 \dots & 0.360 \dots & -0.944 \dots \\ 0.307 \dots & 0.190 \dots & -0.497 \dots \\ -0.139 \dots & -0.086 \dots & 0.226 \dots \end{pmatrix}$. Hence, $\min\{(P_2)_{33} - (P_2)_{23}, (P_2)_{11} - (P_2)_{21}\} \approx 0.276$ while $\frac{\sqrt[3]{\lambda_3}}{\sqrt[3]{\lambda_3} - \sqrt[3]{\lambda_2}} \approx 0.579$, and therefore, according to Lemma 5, $\sqrt[3]{P}$ does not satisfy the monotonicity conditions. Theorem 7 results in the insight that for whatever odd value $m \geq 3$, $\sqrt[m]{P}$ is not a monotone matrix. This example illustrates that there exist monotone matrices for which none of the roots $\sqrt[m]{P}$ (where $m \in \mathbb{N}(\lambda_3)$) satisfies the monotonicity conditions (6).

4.2 Non-diagonalizable monotone matrices of order 3

For a non-diagonalizable matrix P , there exists a transformation matrix T such that $P = T \times J \times T^{-1}$ with the

Jordan matrix $J = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \lambda & 1 \\ 0 & 0 & \lambda \end{pmatrix}$. Consequently, the matrix P can be expressed as $P = P_1 + \lambda P_\lambda + N_\lambda$ with $P_1 = TI_{11}T^{-1}$, $P_\lambda = T(I_{22} + I_{33})T^{-1}$, $N_\lambda = TI_{23}T^{-1}$, (10)

where I_{ij} denotes the (3×3) matrix with (i, j) th element equal to 1 and all the other elements equal to 0.

For a monotone matrix $P = P_1 + \lambda P_\lambda + N_\lambda$, the eigenvalue λ is nonnegative (according to equation (3)). In the case that $\lambda = 0$ there does not exist a stochastic root of P ([11], Theorem 5). Hence, we know that a non-diagonalizable matrix $P \in \mathbb{M}_3$ with $\lambda = 0$ has no monotone matrix root. In the case that $\lambda > 0$, $\sqrt[m]{P} = P_1 + \lambda^{\frac{1}{m}} P_\lambda + \frac{1}{m} \lambda^{\frac{1}{m}-1} N_\lambda$ is an m th root with all row sums equal to 1 [11], and this for all $m \in \mathbb{N} \setminus \{0\}$. Theorem 9 proves, for a monotone matrix $P = P_1 + \lambda P_\lambda + N_\lambda$ with $\lambda > 0$, that the monotonicity conditions are fulfilled for all m th roots $\sqrt[m]{P}$. The following lemma provides some required properties beforehand.

Lemma 8. *For a non-diagonalizable stochastic matrix $P = P_1 + \lambda P_\lambda + N_\lambda$ of order (3×3) with $\lambda > 0$ and m th root $\sqrt[m]{P} = P_1 + \lambda^{\frac{1}{m}} P_\lambda + \frac{1}{m} \lambda^{\frac{1}{m}-1} N_\lambda$ holds for all $i, j, l \in \{1, 2, 3\}$ and for all $m \in \mathbb{N} \setminus \{0\}$:*

$$(P_\lambda)_{il} - (P_\lambda)_{jl} = \delta_{il} - \delta_{jl}$$

$$(\sqrt[m]{P})_{il} \geq (\sqrt[m]{P})_{jl} \Leftrightarrow (N_\lambda)_{il} - (N_\lambda)_{jl} \geq \lambda \cdot m(\delta_{jl} - \delta_{il}).$$

Proof. By definition of P_1 and P_λ it holds that $P_1 + P_\lambda = I_3$, with I_3 the identity matrix of order (3×3) . In addition, the projection P_1 has all rows equal, and therefore, $(P_\lambda)_{il} - (P_\lambda)_{jl} = \delta_{il} - \delta_{jl}$ for all $i, j, l \in \{1, 2, 3\}$.

Furthermore, $(\sqrt[m]{P})_{il} \geq (\sqrt[m]{P})_{jl}$ is equivalent with

$$(P_1)_{il} + \lambda^{\frac{1}{m}}(P_\lambda)_{il} + \frac{1}{m}\lambda^{\frac{1}{m}-1}(N_\lambda)_{il} \geq (P_1)_{jl} + \lambda^{\frac{1}{m}}(P_\lambda)_{jl} + \frac{1}{m}\lambda^{\frac{1}{m}-1}(N_\lambda)_{jl}$$

and also equivalent with $(N_\lambda)_{il} - (N_\lambda)_{jl} \geq \lambda \cdot m(\delta_{il} - \delta_{jl})$ since all elements in a same column of P_1 are equal and $(P_\lambda)_{il} - (P_\lambda)_{jl} = \delta_{il} - \delta_{jl}$. \square

Theorem 9. For a non-diagonalizable monotone matrix $P = P_1 + \lambda P_\lambda + N_\lambda \in \mathbb{M}_3$ with $\lambda > 0$ and P_1, P_λ , and N_λ as in equation (10), the monotonicity conditions (6) also hold for the matrix roots $\sqrt[m]{P} = P_1 + \lambda^{\frac{1}{m}}P_\lambda + \frac{1}{m}\lambda^{\frac{1}{m}-1}N_\lambda$ for all $m \in \mathbb{N} \setminus \{0\}$.

Proof. Since the monotone matrix P satisfies $p_{33} \geq p_{23}$, it holds for $\lambda > 0$ that $(N_\lambda)_{33} - (N_\lambda)_{23} \geq -\lambda \geq -\lambda \cdot m$ and therefore, $(\sqrt[m]{P})_{33} \geq (\sqrt[m]{P})_{23}$. In a similar way: $(\sqrt[m]{P})_{11} \geq (\sqrt[m]{P})_{21}$.

Furthermore, $p_{23} \geq p_{13}$ and consequently, $(N_\lambda)_{13} - (N_\lambda)_{23} \geq 0$ and $(\sqrt[m]{P})_{23} \geq (\sqrt[m]{P})_{13}$. Similar arguments result in $(\sqrt[m]{P})_{21} \geq (\sqrt[m]{P})_{31}$. \square

Combining all the properties that are presented in this section leads to the conclusions summarized in Table 1, for $P \in \mathbb{M}_3$ and $\sqrt[m]{P}$ defined as

$$\begin{aligned} \sqrt[m]{P} &= P_1 + \sqrt[m]{\lambda_2}P_2 + \sqrt[m]{\lambda_3}P_3 \quad \text{for } P = P_1 + \lambda_2 P_2 + \lambda_3 P_3 \text{ diagonalizable} \\ &= P_1 + \lambda^{\frac{1}{m}}P_\lambda + \frac{1}{m}\lambda^{\frac{1}{m}-1}N_\lambda \quad \text{for } P = P_1 + \lambda P_\lambda + N_\lambda \text{ non-diagonalizable.} \end{aligned}$$

A monotone matrix is discrete embeddable within \mathbb{M}_3 if there exists a matrix root that satisfies the monotonicity conditions and that is simultaneously a stochastic matrix. In this way, the results in [11] (Table 1), in combination with the results in Table 1 of this article provide full information on stochasticity as well as monotonicity of matrix roots for $P \in \mathbb{M}_3$.

Table 1: Properties of $\sqrt[m]{P}$ for $P \in \mathbb{M}_3$ and all possible configurations for the eigenvalue(s) $\lambda_2 \geq \lambda_3$

| | | |
|-------------------------------|-----------------------------------|--|
| P diagonalizable | $\lambda_2 \geq \lambda_3 \geq 0$ | $\sqrt[m]{P} \in \text{MC}_3$ Theorem 6 |
| | $\lambda_2 \geq 0 > \lambda_3$ | $\exists m : \sqrt[m]{P} \in \text{MC}_3 \Leftrightarrow \sqrt[3]{P} \in \text{MC}_3$ Theorem 7 |
| | $0 > \lambda_2 \geq \lambda_3$ | No such monotone matrix P exists (redundant case) Equation (3) |
| P non-diagonalizable | $\lambda > 0$ | $\sqrt[m]{P} \in \text{MC}_3$ Theorem 9 |
| | $\lambda = 0$ | No matrix root of P in \mathbb{M}_3 Theorem 5 in [11] |
| | $\lambda < 0$ | No such monotone matrix P exists (redundant case) Equation (3) |

4.3 Further remarks and examples

In this section, some further remarks are formulated and examples are presented to highlight possible scenarios.

Theorem 6 guarantees for a diagonalizable matrix $P \in \mathbb{M}_3$ with nonnegative eigenvalues that the monotonicity properties (6) also hold for the m th root $\sqrt[m]{P}$. For example, $P = \begin{pmatrix} 0.4 & 0.3 & 0.3 \\ 0.3 & 0.3 & 0.4 \\ 0.1 & 0.1 & 0.8 \end{pmatrix}$ has three distinct positive eigenvalues and the square root $\sqrt{P} = \begin{pmatrix} 0.556 \dots & 0.288 \dots & 0.154 \dots \\ 0.283 \dots & 0.448 \dots & 0.268 \dots \\ 0.057 \dots & 0.062 \dots & 0.879 \dots \end{pmatrix}$ satisfies the monotonicity conditions. Moreover, this root is a stochastic matrix, and therefore, P has a monotone square root and is discrete embeddable within \mathbb{M}_3 .

Fact 4.1. Although $\sqrt[m]{P}$ satisfies the monotonicity conditions for $P \in \mathbb{M}_3$ with positive eigenvalues, $\sqrt[m]{P}$ is not necessarily a monotone matrix.

For example, for $P = \begin{pmatrix} 0.8 & 0.2 & 0 \\ 0.5 & 0.3 & 0.2 \\ 0.1 & 0.4 & 0.5 \end{pmatrix}$, the square root $\sqrt{P} = \begin{pmatrix} 0.854 \dots & 0.167 \dots & -0.022 \dots \\ 0.407 \dots & 0.391 \dots & 0.201 \dots \\ -0.039 \dots & 0.391 \dots & 0.648 \dots \end{pmatrix}$ has not

all its elements nonnegative. In fact, the computation of all square roots of P let conclude that none of the square roots is a stochastic matrix and, therefore, neither a monotone matrix. One can remark that P has three distinct positive eigenvalues, and Theorem 3 is not applicable. In fact, having all eigenvalues positive is not a sufficient condition to be discrete embeddable within the set \mathbb{M}_3 .

Fact 4.2. Theorem 6 proves for a diagonalizable monotone matrix P with nonnegative eigenvalues, the monotonicity properties (6) for a particular m th root, being $\sqrt[m]{P} = T \times \text{diag}(1, \sqrt[m]{\lambda_2}, \sqrt[m]{\lambda_3}) \times T^{-1}$. It is, in general, not the case that the monotonicity properties also hold for any other m th root of $P \in \mathbb{M}_3$.

For example, for the monotone matrix $P = \begin{pmatrix} 0.4 & 0.3 & 0.3 \\ 0.3 & 0.3 & 0.4 \\ 0.1 & 0.1 & 0.8 \end{pmatrix}$, although $\sqrt{P} = T \times \text{diag}(1, \sqrt{\lambda_2}, \sqrt{\lambda_3}) \times T^{-1} \in \mathbb{M}_3$, the stochastic square root $T \times \text{diag}(1, -\sqrt{\lambda_2}, \sqrt{\lambda_3}) \times T^{-1} = \begin{pmatrix} 0.392 \dots & 0.497 \dots & 0.109 \dots \\ 0.481 \dots & 0.194 \dots & 0.323 \dots \\ 0.052 \dots & 0.068 \dots & 0.878 \dots \end{pmatrix}$ does not satisfy the monotonicity conditions.

5 Roots of $(n \times n)$ monotone matrices

5.1 Monotonicity conditions in matrix form

For higher order matrices, it has advantages to express the monotonicity conditions (2) more compact in matrix form. In a similar way, Conlisk defined in [19] necessary and sufficient conditions for a stochastic matrix to be a monotone matrix based on its dominance matrix.

Let us introduce the $(n \times (n - 1))$ matrix S^+ with on its j th column the first j th elements equal to 0 and the other elements equal to 1, and the $((n - 1) \times n)$ matrix S^- with the elements $(S^-)_{ii}$ equal to -1 , the elements $(S^-)_{i,i+1}$ equal to 1, and all other elements equal to 0:

$$S^+ = \begin{pmatrix} 0 & 0 & \dots & 0 \\ 1 & 0 & \dots & 0 \\ 1 & 1 & \dots & 0 \\ \vdots & & & \\ 1 & 1 & \dots & 1 \end{pmatrix} \quad S^- = \begin{pmatrix} -1 & 1 & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & \dots & 0 & 0 & 0 \\ & & & & & \vdots & & \\ 0 & 0 & 0 & 0 & \dots & 0 & -1 & 1 \end{pmatrix}.$$

Multiplying $M \in \mathcal{S}_n$ on the right side with S^+ results in the summations that are part of equation (2), which are then subtracted after multiplying $M \times S^+$ with S^- on the left side. Hence, for all $k, l \in \{1, \dots, n - 1\}$ holds

$$(S^- \times M \times S^+)_{kl} = \sum_{j=l+1}^n m_{k+1,j} - \sum_{j=l+1}^n m_{kj}. \quad (11)$$

Consequently,

$$M \in \text{MC}_n \Leftrightarrow S^- \times M \times S^+ \geq 0. \quad (12)$$

One can remark, for $M \in S_n$, that $S^- \times M \times S^+ = D(M)$, where $D(M)$ is the dominance matrix with elements $(D(M))_{kl} = \sum_{j=1}^l m_{kj} - \sum_{j=1}^l m_{k+1,j}$ as introduced in [19].

5.2 Properties not generalizable from $n \leq 3$ to $n > 3$

It is important to be aware that some properties, proven in Sections 3 and 4, no longer hold for $(n \times n)$ monotone matrices with $n > 3$.

Each (2×2) stochastic matrix has all its eigenvalues real-valued. Hence, the same property holds for all matrices in \mathbb{M}_2 . Besides, a monotone matrix of order (3×3) has all its eigenvalues real-valued according to Theorem 2. Nevertheless, this property does not hold any longer for higher order monotone matrices:

Fact 5.1. A monotone matrix of order $(n \times n)$ with $n > 3$, has not necessarily all eigenvalues real-valued.

For example, $P = \begin{pmatrix} 0.2 & 0 & 0.8 & 0 \\ 0.2 & 0 & 0 & 0.8 \\ 0 & 0.1 & 0.1 & 0.8 \\ 0 & 0 & 0 & 1 \end{pmatrix}$ has 1 and 0.3652 as real eigenvalues and $-0.0326 + 0.2068i$ and $-0.0326 - 0.2068i$ as complex eigenvalues.

For each (2×2) monotone matrix P , the matrix root $\sqrt[n]{P}$ is a monotone matrix (according to Theorem 1). For a monotone matrix P of order (3×3) with positive eigenvalues, Theorems 6 and 9 prove that the monotonicity conditions are fulfilled for the root $\sqrt[n]{P}$.

Fact 5.2. The monotonicity properties do not necessarily hold for $\sqrt[n]{P}$ in case P is a monotone matrix of order $(n \times n)$ with $n > 3$.

For example, $P = \begin{pmatrix} 0.5 & 0.2 & 0.1 & 0.2 \\ 0.2 & 0.4 & 0.2 & 0.2 \\ 0.1 & 0.2 & 0.4 & 0.3 \\ 0.1 & 0.2 & 0.1 & 0.6 \end{pmatrix}$ has all eigenvalues real-valued and positive. Nevertheless, the

stochastic square root

$$\sqrt{P} = \begin{pmatrix} 0.685 \dots & 0.138 \dots & 0.055 \dots & 0.120 \dots \\ 0.146 \dots & 0.585 \dots & 0.156 \dots & 0.112 \dots \\ 0.053 \dots & 0.138 \dots & 0.603 \dots & 0.205 \dots \\ 0.053 \dots & 0.138 \dots & 0.055 \dots & 0.752 \dots \end{pmatrix}$$

does not satisfy the monotonicity conditions.

The discrete embedding problem and investigating monotone matrix roots for general $(n \times n)$ monotone matrices with $n > 3$ is not easy. There are some alternative approaches to make progress in studying monotone matrix roots of $(n \times n)$ monotone matrices.

In case a monotone matrix P is continuous embeddable within the set of stochastic matrices and a generator G does exist that satisfies equation (4), then $P = e^G$ is continuous embeddable within the set of monotone matrices. Hence, the matrix roots $e^{G/m}$ are monotone and P is discrete embeddable within \mathbb{M}_n . In applications, the transition matrix of a monotone Markov system under study is often the result of estimated transition probabilities based on an available dataset. Consequently, there is anyway a discrepancy between the estimated and the theoretical transition matrix. Therefore, if P is not continuous embeddable, then it is acceptable to replace P by an arbitrarily close approximation that is continuous embeddable [27] and that results in approximations for the roots of P , for which the monotonicity conditions can be examined.

Alternatively, since the set of diagonalizable monotone matrices is dense within \mathbb{M}_n [28], a monotone transition matrix that is not diagonalizable can be approximated by an arbitrarily close diagonalizable matrix of \mathbb{M}_n . Having insights regarding the properties of the roots of diagonalizable monotone matrices is then useful and that is where the following section focuses on.

5.3 Diagonalizable monotone matrices

In this section, we investigate roots and embedding conditions for diagonalizable monotone matrices of order $(n \times n)$.

Lemma 10. *For a diagonalizable matrix $A = (a_{ij}) \in S_n$ with eigenvalues $1 = \mu_1, \mu_2, \dots, \mu_n$ and corresponding projections A_1, A_2, \dots, A_n holds*

$$A \in \text{MC}_n \Leftrightarrow \sum_{s=2}^{s=n} \mu_s (S^- \times A_s \times S^+) \geq 0.$$

Proof. The diagonalizable matrix A can be expressed as $A = A_1 + \mu_2 A_2 + \dots + \mu_n A_n$. Since the projection A_1 has all its rows equal, holds $S^- \times A_1 \times S^+ = 0$. Hence, $S^- \times A \times S^+ \geq 0$ if and only if $\sum_{s=2}^{s=n} \mu_s (S^- \times A_s \times S^+) \geq 0$, which proofs the lemma according to equation (12). \square

From the discussion in Section 4, we know that, for a (3×3) diagonalizable monotone matrix P with nonnegative eigenvalues, the roots $\sqrt[3]{P}$ satisfy the monotonicity conditions. On the other hand, the example in Fact 5.2 demonstrates that this property does not hold any longer for $n > 3$. The question, therefore, is now under what conditions the result can be (partially) generalized to higher-order monotone matrices. Therefore, we consider a diagonalizable matrix $P = P_1 + \lambda_2 P_2 + \dots + \lambda_n P_n \in \mathbb{M}_n$, with nonnegative eigenvalues $1 = \lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n \geq 0$ and corresponding projections P_1, P_2, \dots, P_n , and examine the monotonicity conditions of the m th root

$$\sqrt[m]{P} = P_1 + \sqrt[m]{\lambda_2} P_2 + \dots + \sqrt[m]{\lambda_n} P_n.$$

By introducing for $k, l \in \{1, \dots, n-1\}$ the function

$$f_{kl}(x) = \sum_{s=2}^{s=n} \lambda_s^x (S^- \times P_s \times S^+)_{kl}, \quad (13)$$

we have that

$$f_{kl}\left(\frac{1}{m}\right) = \sum_{s=2}^{s=n} \sqrt[m]{\lambda_s} (S^- \times P_s \times S^+)_{kl} = (S^- \times \sqrt[m]{P_s} \times S^+)_{kl} = \sum_{j=l+1}^n (\sqrt[m]{P})_{k+1,j} - \sum_{j=l+1}^n (\sqrt[m]{P})_{kj} \quad (14)$$

according to equation (11).

Hence, by using Lemma 10, the monotonicity conditions (2) can be expressed as follows:

$$\sqrt[m]{P} \in \text{MC}_n \Leftrightarrow f_{kl}\left(\frac{1}{m}\right) \geq 0 \quad \forall k, l \in \{1, \dots, n-1\}. \quad (15)$$

Since the matrix $P = P_1 + \lambda_2 P_2 + \dots + \lambda_n P_n$ and the identity matrix $I_n = P_1 + P_2 + \dots + P_n$ are both monotone, holds

$$f_{kl}(1) \geq 0 \quad \text{and} \quad f_{kl}(0) \geq 0 \quad \forall k, l \in \{1, \dots, n-1\}. \quad (16)$$

Moreover, the specificity of the identity matrix results in $S^- \times I_n \times S^+ = I_{n-1}$, and therefore,

$$f_{kl}(0) = \delta_{kl}. \quad (17)$$

According to equation (15), in examining the monotonicity conditions, the sign of the function $f_{kl}(x)$ and, therefore, its zero points are of importance. Since the function $f_{kl}(x)$ is a sum of the exponential functions λ_s^x , the number of positive solutions of $f_{kl}(x) = 0$ is at most equal to the number of sign changes in the sequence of coefficients in descending order of the basis $\lambda_2 \geq \dots \geq \lambda_n$ of the exponential functions [29].

Hence, for $k, l \in \{1, \dots, n-1\}$, the number of sign changes in the sequence

$$(S^- \times P_2 \times S^+)_{kl}, (S^- \times P_3 \times S^+)_{kl}, \dots, (S^- \times P_n \times S^+)_{kl} \quad (18)$$

provides useful information regarding the number of positive zero points of the function $f_{kl}(x)$.

Let us introduce the notations

$$x_{kl}^* = \max\{x \in [0, 1] | f_{kl}(x) = 0\} \quad \text{and} \quad x^* = \max\{x_{kl}^* | k, l \in \{1, \dots, n-1\}\} \quad (19)$$

in order to be able to formulate in Theorem 11 sufficient conditions that guarantee that the matrix root $\sqrt[m]{P}$ satisfies the monotonicity conditions.

Theorem 11. *In case $x^* \leq \frac{1}{2}$, where x^* is accordingly equation (19), then for all $m \in \mathbb{N}$, $m \geq 2$ with $\frac{1}{m} \geq x^*$ holds that $\sqrt[m]{P} \in \text{MC}_n$.*

Proof. In case $x^* \leq \frac{1}{2}$, for arbitrary $k, l \in \{1, \dots, n-1\}$, the continuous function $f_{kl}(x)$ (as defined in equation (13)) has no zero points in $[x^*, 1]$ and is positive for $x = 1$ (according to equation (16)). Consequently, $f_{kl}(x)$ is nonnegative on $[x^*, 1]$ so that, in particular, for all $m \in \mathbb{N}$, $m \geq 2$, with $\frac{1}{m} \geq x^*$ holds that $f_{kl}\left(\frac{1}{m}\right) \geq 0$. Hence, by equation (15), $\sqrt[m]{P} \in \text{MC}_n$. \square

Theorem 12. *In case for the diagonalizable monotone matrix P with projections P_2, P_3, \dots, P_n , there is none or only one sign change in the sequence*

$$(S^- \times P_2 \times S^+)_{kl}, (S^- \times P_3 \times S^+)_{kl}, \dots, (S^- \times P_n \times S^+)_{kl}$$

for $k, l \in \{1, \dots, n-1\}$, then for all $m \in \mathbb{N}$, $m \geq 2$, the m th root matrix $\sqrt[m]{P}$ satisfies the (k, l) th monotonicity condition $\sum_{j=l+1}^n (\sqrt[m]{P})_{k+1,j} - \sum_{j=l+1}^n (\sqrt[m]{P})_{kj} \geq 0$.

Proof. In case there is none or only one sign change in the sequence (18), then the function $f_{kl}(x)$ has at most one zero point in $[0, 1]$. Moreover, $f_{kl}(0)$ and $f_{kl}(1)$ are both nonnegative according to equation (16). Consequently, $f_{kl}(x) \geq 0$ for all $x \in [0, 1]$. In particular, $f_{kl}\left(\frac{1}{m}\right) \geq 0$ and the theorem follows from equation (14). \square

The result of Theorem 12 is useful in studying the existence of monotone roots. For example, for

$$P = \begin{pmatrix} 0.5 & 0.2 & 0.1 & 0.2 \\ 0.2 & 0.4 & 0.2 & 0.2 \\ 0.1 & 0.2 & 0.4 & 0.3 \\ 0.1 & 0.2 & 0.1 & 0.6 \end{pmatrix},$$

we have already mentioned in Section 5.2 that \sqrt{P} does not satisfy the monotonicity conditions. The question that can be stated then is whether there exists a value $m > 2$ such that the m th root $\sqrt[m]{P}$ satisfies the monotonicity conditions. By computing

$$\begin{aligned} S^- \times P_2 \times S^+ &= \begin{pmatrix} 0.5 & 0.5 & 0.5 \\ 0.5 & 0.5 & 0.5 \\ 0 & 0 & 0 \end{pmatrix} \\ S^- \times P_3 \times S^+ &= \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \\ S^- \times P_4 \times S^+ &= \begin{pmatrix} 0.5 & -0.5 & 0.5 \\ -0.5 & 0.5 & -0.5 \\ 0 & 0 & 0 \end{pmatrix}, \end{aligned}$$

one can note that the sequence (18) has two sign changes for $k = 1$ and $l = 3$ and zero or one sign change for all other pairs (k, l) . Hence, according to Theorem 12, for all m th roots $\sqrt[m]{P}$, the (k, l) th monotonicity condition is fulfilled for all $(k, l) \neq (1, 3)$. On the other hand, $f_{1,3}(0) = f_{1,3}(1) = 0$ and $f_{1,3}\left(\frac{1}{2}\right) < 0$. Hence, $f_{1,3}(x) < 0$ for all $x \in]0, 1[$ since the function $f_{1,3}(x)$ has at most two zero-points in $[0, 1]$. Consequently, one can conclude that none of the matrix roots $\sqrt[m]{P}$ satisfies the $(1, 3)$ th monotonicity condition, and therefore, none of the roots $\sqrt[m]{P}$ is a monotone matrix.

5.4 Block diagonal monotone matrices

In case of a block diagonal Markov model with n states, the transition matrix $P = \text{diag}(B_1(P), \dots, B_k(P))$ is of order $(n \times n)$ with blocks $B_i(P)$ of order $(n_i \times n_i)$, satisfying $\sum_{i=1}^k n_i = n$, and is of the form:

$$P = \text{diag}(B_1(P), \dots, B_k(P)) = \begin{pmatrix} B_1(P) & O & \dots & O \\ O & B_2(P) & \ddots & \vdots \\ \vdots & \ddots & & O \\ O & \dots & O & B_k(P) \end{pmatrix}.$$

The nature of the monotonicity conditions (1) results for a block diagonal matrix $P = \text{diag}(B_1(P), \dots, B_k(P))$ in:

$$P = \text{diag}(B_1(P), \dots, B_k(P)) \in \mathbb{M}_n \Leftrightarrow B_i(P) \in \mathbb{M}_{n_i} \quad \forall i \in \{1, \dots, k\}.$$

Therefore, for a monotone matrix $P = \text{diag}(B_1(P), \dots, B_k(P))$, equation (3) applies for each block $B_i(P)$ and, consequently, $\text{tr}(P) = \text{tr}(B_1(P)) + \dots + \text{tr}(B_k(P)) \geq k$. This means that the trace of all monotone matrices is at least equal to 1, and that for those that are block diagonal, the trace is even at least equal to the number of blocks. The following theorem formulates this characterization of the trace.

Theorem 13. *A block diagonal monotone matrix P satisfies $\text{tr}(P) \geq k$, where k is the number of blocks.*

Furthermore, $A = \text{diag}(B_1(A), \dots, B_k(A))$ is an m th root matrix of P if and only if for all $i \in \{1, \dots, k\}$ holds that $B_i(A)$ is an m th root of $B_i(P)$. Therefore, in case the blocks $B_i(P)$ are of order (2×2) or (3×3) , the specific properties presented in Sections 3 and 4 are helpful in examining matrix roots of the monotone matrix $P = \text{diag}(B_1(P), \dots, B_k(P))$. In particular, a block diagonal monotone matrix $P = \text{diag}(B_1(P), \dots, B_k(P))$ with $n_i = 2$ for all i , has, for all $m \in \mathbb{N} \setminus \{0\}$, $A = \text{diag}(\sqrt[m]{B_1(P)}, \dots, \sqrt[m]{B_k(P)})$ as monotone m th root, where $\sqrt[m]{B_1(P)}, \dots, \sqrt[m]{B_k(P)}$ are as described in Theorem 1. In case a block $B_i(P)$ is of order $n > 3$, Theorems 11 and 12 are useful in examining the monotonicity properties of $\sqrt[m]{B_i(P)}$.

6 Further research questions

Within the set of monotone matrices, the discrete embedding problem is completely clarified for the case of (2×2) matrices. Each monotone matrix is embeddable within the set \mathbb{M}_2 . Moreover, each (2×2) monotone matrix has a monotone m th root, for all $m \in \mathbb{N} \setminus \{0\}$ [22]. Within the set \mathbb{M}_3 holds, according to Theorems 6 and 9, that each monotone matrix with positive eigenvalues has an m th root that satisfies the monotonicity conditions. For $n > 3$, roots within \mathbb{M}_n are investigated for two important subsets of monotone matrices: for diagonalizable matrices in Section 5.3 and for block diagonal matrices in Section 5.4. For further research, it would be interesting to investigate matrix roots within \mathbb{M}_n for more general $(n \times n)$ monotone matrices.

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