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Tridiagonal and Pentadiagonal Doubly Stochastic Matrices

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Tridiagonal doubly stochastic matrices arise in the literature in a number of areas, in particular with respect to the study of Markov chains and in majorization theory. The facial structure of Ω_n^t , with a connection to majorization, is explored in [9]. In [12], the author develops relations involving sums of Jensen functionals to compare tuples of vectors; a tridiagonal doubly stochastic matrix is used to demonstrate their results. In the study of mixing rates for Markov chains the assumption of symmetry in the transition matrix is sometimes seen, as in [5]. Other times, the Markov chain is assumed to be a path [6, 4] leading to a tridiagonal transition matrix. The properties of symmetric doubly stochastic matrices are explored in [13], where majorization relations are given for the eigenvalues. Properties related to the facial structure of Ω_n^t can be found in [8, 7]. In the former, alternating parity sequences are used to express the number of vertices of a given face, and in the latter, the number of q -faces of Ω_n^t for arbitrary n is determined for $q = 1, 2, 3$.

We are interested in positivity conditions for tridiagonal doubly stochastic matrices. A stronger condition than positive semidefiniteness, known as complete positivity, has applications in a variety of areas of study, including block designs, maximin efficiency-robust tests, modelling DNA evolution, and more [3, Chapter 2], as well as recent use in mathematical optimization and quantum information theory (see [11] and the references therein).

With this motivation in mind, we study the positivity (in various forms) of tridiagonal doubly stochastic matrices. The paper is organized as follows. In Section 2.1, we characterize when a tridiagonal doubly stochastic matrix is positive semidefinite based on its nonzero entries, specifically the entries of its sub- and super-diagonal, and we study the eigenvalues of tridiagonal doubly stochastic matrices. Although it is NP-hard to determine if a given matrix is completely positive [10], in Section 2.2 we provide a construction that is sufficient to show that a given symmetric tridiagonal (not necessarily doubly stochastic) matrix is completely positive. We provide a number of examples illustrating the utility of this construction, and ultimately prove that positive definiteness and complete positivity coincide for these matrices.

As a natural extension, we generalize many of our results to symmetric pentadiagonal matrices in Section 3. While a construction analogous to that for the tridiagonal setting works in the pentadiagonal setting, we also provide an alternate, more involved, construction that works in many cases when the original construction does not.

2. TRIDIAGONAL DOUBLY STOCHASTIC MATRICES

2.1. Basic Properties. One can ask under what conditions is a tridiagonal doubly stochastic matrix A positive semidefinite. It is known that a symmetric diagonally dominant matrix A with non-negative diagonal entries is positive semidefinite. Thus, in our case, if

$$(1) \quad b_{i-1} + b_i \leq 0.5$$

for all $i = 1, 2, \dots, n$, with $b_0 = b_n = 0$, then A is diagonally dominant, and hence A is positive semidefinite. So (1) is sufficient for positive semidefiniteness of a tridiagonal doubly stochastic matrix. The following result shows that (1) is also necessary.

Lemma 1. *Let A be a tridiagonal doubly stochastic matrix. Then A is positive semidefinite if and only if (1) holds for all $i = 1, 2, \dots, n$, with $b_0 = b_n = 0$.*

Proof. The sufficiency proof is discussed above. For the necessity of (1), we note that by the Gershgorin circle theorem, each eigenvalue of A lies in at least one Gershgorin disk. Using the notation above, the disks are centered at a_i and have radius $b_{i-1} + b_i$. Thus if we want

the eigenvalues to be non-negative, we need $a_i - b_{i-1} - b_i \geq 0$. Subbing in $a_i = 1 - b_{i-1} - b_i$ (the assumption that A is doubly stochastic) and rearranging yields (1). \square

We now present some results related to the eigenvalues of tridiagonal doubly stochastic matrices, which can be deduced from standard facts in the literature.

If λ is an eigenvalue of a stochastic matrix, it is well-known that $\lambda \in \mathbb{C}$ such that $|\lambda| \leq 1$. In our context, we note that if λ is an eigenvalue of a tridiagonal doubly stochastic matrix A , then $-1 \leq \lambda \leq 1$. The fact that $\lambda \in \mathbb{R}$ follows immediately from the fact that a tridiagonal doubly stochastic matrix is symmetric.

Lemma 2. *Let A be a tridiagonal doubly stochastic matrix. The eigenvalues of A all lie in $[-1, 1]$.*

In fact, we can say something stronger: The set of all possible eigenvalues of tridiagonal doubly stochastic matrices is $[-1, 1]$.

Proposition 1. *Let $n \geq 2$. λ is an eigenvalue of an $n \times n$ tridiagonal doubly stochastic matrix if and only if $\lambda \in [-1, 1]$.*

Proof. Suppose $\lambda \in [-1, 1]$ is arbitrary. The 2×2 tridiagonal doubly stochastic matrix $A = \begin{pmatrix} a & b \\ b & a \end{pmatrix}$ with $a + b = 1$, $a \in [0, 1]$, has eigenvalues 1 and $2a - 1$. So choose a such that $2a - 1 = \lambda$, i.e. $a = (\lambda + 1)/2$. Then λ is an eigenvalue of the constructed matrix A . For $n > 2$, note that we can construct an $n \times n$ tridiagonal doubly stochastic matrix via $A \oplus B$, where B is an $(n - 2) \times (n - 2)$ tridiagonal doubly stochastic matrix, and the constructed matrix $A \oplus B$ has λ as an eigenvalue (if v is an eigenvector corresponding to λ for the matrix A , then $v \oplus \mathbf{0}_{n-2}$, where $\mathbf{0}_{n-2}$ is the $(n - 2)$ -dimensional zero vector, is an eigenvector corresponding to λ for $A \oplus B$). Thus one can construct a tridiagonal doubly stochastic matrix of arbitrary size having the prescribed eigenvalue λ .

The converse follows from Lemma 2. \square

2.2. Complete Positivity.

Definition 1. *An $n \times n$ real matrix A is completely positive if it can be decomposed as $A = VV^T$, where V is an $n \times k$ entrywise non-negative matrix, for some k .*

Equivalently, one can define A to be completely positive provided $A = \sum_{i=1}^k v_i v_i^T$, where v_i are entrywise non-negative vectors (namely, the columns of V).

Completely positive matrices are positive semidefinite and symmetric entrywise non-negative; such matrices are called *doubly non-negative*. Doubly non-negative matrices are completely positive for $n \leq 4$, while doubly non-negative matrices that are not completely positive exist for all $n \geq 5$; see [1] and the references therein. In other words, the set of all completely positive matrices forms a strict subset of the set of all doubly non-negative matrices for $n \geq 5$.

We outline below a construction producing the completely positive decomposition $A = \sum_i v_i v_i^T$, which can be found by assuming that, since A is tridiagonal, each v_i should have only two nonzero entries (the i -th and $(i + 1)$ -th entries), and brute-force solving for these entries from the equation $A = VV^T$; these values can also be found somewhat indirectly, assuming our initial condition is zero, through a construction of pairwise completely positive matrices in [11, Theorem 4] by taking both matrices to be A .

For a given $n \times n$ symmetric tridiagonal matrix A , define the set $\{v_i\}_{i=0}^n$ of $n + 1$ n -dimensional vectors where the j -th component of v_i , denoted $(v_i)_j$, is recursively defined by

$$(2) \quad (v_i)_j = \begin{cases} \sqrt{a_i - ((v_{i-1})_i)^2} & j = i \\ b_i / (v_i)_i & j = i + 1 \\ 0 & \text{otherwise} \end{cases}$$

with initial condition $v_0 = (a_0 \ 0 \ \dots \ 0)^T$. This construction yields

$$\begin{aligned} v_1 &= \left(\sqrt{a_1 - a_0^2} \quad \frac{b_1}{\sqrt{a_1 - a_0^2}} \quad 0 \quad \dots \quad 0 \right)^T \\ v_2 &= \left(0 \quad \sqrt{a_2 - \frac{b_1^2}{a_1 - a_0^2}} \quad \frac{b_2}{\sqrt{a_2 - \frac{b_1^2}{a_1 - a_0^2}}} \quad 0 \quad \dots \quad 0 \right)^T \\ v_3 &= \left(0 \quad 0 \quad \sqrt{a_3 - \frac{b_2^2}{a_2 - \frac{b_1^2}{a_1 - a_0^2}}} \quad \frac{b_3}{\sqrt{a_3 - \frac{b_2^2}{a_2 - \frac{b_1^2}{a_1 - a_0^2}}}} \quad 0 \quad \dots \quad 0 \right)^T, \text{ etc.} \end{aligned}$$

The constant a_0 must satisfy $a_0 \geq 0$, however it is worth noting that certain values of a_0 (the most obvious case being $a_0^2 = a_1$) can lead to some of the v_i vectors being ill-defined.

Proposition 2. *Let A be an $n \times n$ symmetric tridiagonal matrix and $a_0 \geq 0$. Then $A = \sum_{i=1}^n v_i v_i^T$ with the v_i as defined in Equation (2). Assuming that all the components for each v_i are non-negative numbers, then A is completely positive.*

We note that if A is entrywise non-negative, which includes the case of A being doubly stochastic, then if the entries of the v_i are all real, then they are automatically non-negative.

Proof. Consider a symmetric tridiagonal matrix A such that the vectors in Equation (2) are well-defined. Let $V_i = v_i v_i^T$ for $i = 0, 1, \dots, n$ and $\tilde{A} = \sum_{i=0}^n V_i$. We wish to show that $\tilde{A} = A$. From the definition of the v_i given in Equation (2), each V_i is tridiagonal with only up to four nonzero entries and so \tilde{A} itself is tridiagonal. Now, consider a component $\tilde{a}_{j,j+1}$ of \tilde{A} , where $j = 1, 2, \dots, n - 1$. The only V_i that will have a nonzero entry in the $(j, j + 1)$ -th component will be V_j as v_j is the only vector with both the j and $(j + 1)$ -th components being nonzero. The $(j, j + 1)$ -th component of V_j is in fact b_j and so $\tilde{a}_{j,j+1} = b_j$. By symmetry, we also have $\tilde{a}_{j+1,j} = b_j$. Now consider a component on the diagonal of \tilde{A} : \tilde{a}_{jj} , where $j = 1, 2, \dots, n$. The only V_i that have nonzero entries in the (j, j) -th component will be V_j and V_{j-1} , with respective values $a_j - ((v_{j-1})_j)^2$ and $((v_{j-1})_j)^2$. Clearly then $\tilde{a}_{jj} = a_j$ for $j = 1, 2, \dots, n$. Therefore $A = \tilde{A} = \sum_{i=1}^n v_i v_i^T$; i.e. A is completely positive. \square

Example 1. *Consider the 5×5 case, which is the first (in terms of smallest dimension) non-trivial case. For the matrices*

$$A = \begin{pmatrix} 3/4 & 1/4 & 0 & 0 & 0 \\ 1/4 & 1/2 & 1/4 & 0 & 0 \\ 0 & 1/4 & 1/2 & 1/4 & 0 \\ 0 & 0 & 1/4 & 1/2 & 1/4 \\ 0 & 0 & 0 & 1/4 & 3/4 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} 7/9 & 2/9 & 0 & 0 & 0 \\ 2/9 & 5/9 & 2/9 & 0 & 0 \\ 0 & 2/9 & 7/9 & 0 & 0 \\ 0 & 0 & 0 & 8/9 & 1/9 \\ 0 & 0 & 0 & 1/9 & 8/9 \end{pmatrix}$$

our construction with $a_0 = 0$ gives $A = VV^T$ and $B = WW^T$ where

$$V = \begin{pmatrix} \frac{1}{2}\sqrt{3} & 0 & 0 & 0 & 0 \\ \frac{1}{2\sqrt{3}} & \frac{1}{2}\sqrt{\frac{5}{3}} & 0 & 0 & 0 \\ 0 & \frac{1}{2}\sqrt{\frac{3}{5}} & \frac{1}{2}\sqrt{\frac{7}{5}} & 0 & 0 \\ 0 & 0 & \frac{1}{2}\sqrt{\frac{5}{7}} & \frac{3}{2\sqrt{7}} & 0 \\ 0 & 0 & 0 & \frac{1}{6}\sqrt{7} & \frac{1}{3}\sqrt{5} \end{pmatrix} \quad \text{and} \quad W = \begin{pmatrix} \frac{1}{3}\sqrt{7} & 0 & 0 & 0 & 0 \\ \frac{2}{3\sqrt{7}} & \frac{1}{3}\sqrt{\frac{31}{7}} & 0 & 0 & 0 \\ 0 & \frac{2}{3}\sqrt{\frac{7}{31}} & \sqrt{\frac{21}{31}} & 0 & 0 \\ 0 & 0 & 0 & \frac{2}{3}\sqrt{2} & 0 \\ 0 & 0 & 0 & \frac{1}{6\sqrt{2}} & \frac{1}{2}\sqrt{\frac{7}{2}} \end{pmatrix}.$$

Therefore the matrices A and B are completely positive. Note that V and W should be 6×6 matrices; however, the selection of $a_0 = 0$ forces v_0 to be the zero vector and as such the first column of both V and W is all zeroes, so can be omitted. For this reason, choosing $a_0 = 0$ often leads to a much simpler decomposition.

It is important to emphasise here that a decomposition proving that a matrix A is completely positive is in general not unique. In particular, the choice of a_0 can lead to different decompositions, assuming they are still well-defined. For example, if we had instead chosen $a_0 = 3/4$, the matrix

$$\tilde{W} = \begin{pmatrix} \frac{3}{4} & \frac{1}{12}\sqrt{31} & 0 & 0 & 0 & 0 \\ 0 & \frac{8}{3\sqrt{31}} & \frac{1}{3}\sqrt{\frac{91}{31}} & 0 & 0 & 0 \\ 0 & 0 & \frac{2}{3}\sqrt{\frac{31}{91}} & \sqrt{\frac{57}{91}} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{2}{3}\sqrt{2} & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{6\sqrt{2}} & \frac{1}{2}\sqrt{\frac{7}{2}} \end{pmatrix}$$

works in the decomposition of B .

If our matrix is in block form but our decomposition does not work, we may employ the technique illustrated in the example below: treating each block separately.

Example 2. Consider the matrix

$$C = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1/2 & 1/2 & 0 & 0 \\ 0 & 1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 0 & 1/2 & 1/2 \\ 0 & 0 & 0 & 1/2 & 1/2 \end{pmatrix}.$$

Since we have $b_1 = 0$ this gives $(v_1)_2 = 0$. Therefore we also have $(v_3)_3 = \sqrt{a_3 - \frac{b_3^2}{a_2}} = \sqrt{1/2 - 1/2} = 0$. Hence, regardless of our choice of a_0 the component $(v_3)_4$ will never be well-defined. To get around this fact consider C as the block matrix

$$C = \begin{pmatrix} C_1 & 0_{3,2} \\ 0_{2,3} & C_2 \end{pmatrix}.$$

where $0_{n,m}$ denotes the $n \times m$ all-zeros matrix and

$$C_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1/2 & 1/2 \\ 0 & 1/2 & 1/2 \end{pmatrix} \quad \text{and} \quad C_2 = \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}.$$

The matrices C_1 and C_2 on the other hand we have no issues with decomposing. Choosing $a_0 = 0$ we obtain

$$V_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 \end{pmatrix} \quad \text{and} \quad V_2 = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 \end{pmatrix}$$

where $C_1 = V_1 V_1^T$ and $C_2 = V_2 V_2^T$. Therefore

$$V = \begin{pmatrix} V_1 & 0_{3,2} \\ 0_{2,3} & V_2 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 \end{pmatrix}$$

where $C = VV^T$ and hence C is completely positive.

Definition 2. Let A be an $n \times n$ matrix. A is said to be reducible if it can be transformed via row and column permutations to a block upper triangular matrix, with block sizes $< n$. A is irreducible if it is not reducible.

Note that in the context of tridiagonal doubly stochastic matrices, irreducibility is equivalent to $b_i > 0$ for all $i = 1, \dots, n$, i.e. that A cannot be written as the direct sum of smaller tridiagonal doubly stochastic matrices. When considering whether or not a tridiagonal doubly stochastic matrix A is completely positive, we may assume A is irreducible. Indeed, if A were a direct sum of smaller doubly stochastic matrices—implying that some $b_i = 0$ —we could consider these smaller doubly stochastic matrices separately. The V corresponding to A in the decomposition would have the same direct sum structure: it would be the direct sum of the V 's corresponding to the smaller doubly stochastic matrices. If some $b_i = 0$, then the corresponding v_i only has one nonzero element. B in Example 1 is a direct sum of two doubly stochastic matrices and C in Example 2 is a direct sum of three doubly stochastic matrices.

The decomposition given by Equation (2) leads to the following result.

Proposition 3. Let A be a tridiagonal doubly stochastic matrix. If A is positive definite, then A is completely positive.

Proof. Sylvester's criterion tells us that for a real symmetric matrix A , positive definiteness is equivalent to all leading principal minors of A being positive.

Note that all square roots in the denominators of the entries in Equation (2) being well-defined with $a_0 = 0$ imply that all leading principal minors are positive. Indeed, taking $a_0 = 0$ in the construction of Equation (2), we find the following. For v_1 to be well-defined, we have $a_1 > 0$, which is the 1×1 leading principal minor.

For v_2 to be well-defined, we have $a_2 - \frac{b_1^2}{a_1} > 0$, which is equivalent to $a_1 a_2 - b_1^2 > 0$, which is the 2×2 leading principal minor.

For v_3 to be well-defined, we have $a_3 - \frac{b_2^2}{a_2 - \frac{b_1^2}{a_1}} > 0$, which is equivalent to $a_1 a_2 a_3 - a_3 b_1^2 - a_1 b_2^2 > 0$, which is the 3×3 leading principal minor.

Continuing in this manner, the result follows. \square

We are now in a position to discuss the relationship between positive semidefiniteness and complete positivity for tridiagonal doubly stochastic matrices.

It is clear that if a matrix A is completely positive, then it is automatically positive semidefinite. Taussky's theorem [14, Theorem II] allows us to use the eigenvalues of a given tridiagonal doubly stochastic matrix to characterize the converse statement.

Theorem 1. (*Taussky's Theorem*) *Let A be an $n \times n$ irreducible matrix. An eigenvalue of A cannot lie on the boundary of a Gershgorin disk unless it lies on the boundary of every Gershgorin disk.*

Equivalently, Taussky's theorem states that if A is an irreducible, diagonally dominant matrix with at least one inequality of the diagonal dominance being strict (in the context of tridiagonal doubly stochastic matrices, this means that (1) holds with strict inequality for at least one i), then A is nonsingular. This is in fact the original formulation of the theorem in [14].

Proposition 4. *Let A be an $n \times n$ irreducible tridiagonal doubly stochastic matrix. If $n \geq 3$ and A is positive semidefinite, then A is positive definite or, equivalently, A is nonsingular.*

Proof. If A is positive semidefinite, then according to Lemma 1, $b_i + b_{i+1} \leq 0.5$ for all $i = 0, 1, 2, \dots, n$ with $b_0 = b_n = 0$. Suppose 0 is an eigenvalue of A , then by Gershgorin circle theorem, there exists some i such that $b_i + b_{i+1} = 0.5$ meaning that 0 is an eigenvalue on the boundary of a disk, so by Taussky's Theorem, every disk must have boundary at 0; that is, $b_i + b_{i+1} = 0.5$ for all i . We have $b_1 = 0.5$, which makes $b_2 = 0$, which contradicts with the assumption that A is irreducible. \square

Note that the tridiagonal doubly stochastic matrix $\begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}$ is the only 2×2 tridiagonal doubly stochastic matrix that is positive semidefinite, without being positive definite (that is, it is the only 2×2 positive semidefinite tridiagonal doubly stochastic matrix with zero as an eigenvalue). One can see this from (1) and the equivalent formulation of Taussky's theorem. One can verify that it is completely positive with $V = (1/\sqrt{2}, 1/\sqrt{2})^T$.

A number of corollaries follow from Proposition 4.

Corollary 1. *Let A be an $n \times n$ tridiagonal doubly stochastic matrix with $n \geq 3$. If A is positive semidefinite, with zero as an eigenvalue, then A must be reducible with at least one block of the form $\begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}$.*

In light of the following corollary, we note that for tridiagonal doubly stochastic matrices, the notions of completely positive and positive semidefinite coincide. This is a more general statement than our previous Proposition 3. This result appears to be known (e.g. it is mentioned in [9, Section 3] that diagonally dominant tridiagonal doubly stochastic matrices are completely positive), yet we are unaware of a proof in the literature. Given some subtleties in, and the length of, the proof, we have provided the details herein, which culminate in the corollary below. We note that [2, Example 2] states that all tridiagonal doubly stochastic matrices are completely positive, which is not true in general without the assumption of positive semidefiniteness.

Corollary 2. *Let A be an $n \times n$ tridiagonal doubly stochastic matrix. If A is positive semidefinite, then A is completely positive.*

for the $n \geq 3$ cases.

Proposition 5. *Let $n \geq 3$. λ is an eigenvalue of an $n \times n$ symmetric pentadiagonal doubly stochastic matrix if and only if $\lambda \in [-1, 1]$.*

3.2. Complete Positivity. We now provide a construction similar to that for tridiagonal doubly stochastic matrices, to provide a sufficient condition for when a symmetric pentadiagonal doubly stochastic matrix A is completely positive. Define the set $\{v_i\}_{i=-1}^n$ of $n+2$ n -dimensional vectors where the j -th component of v_i , denoted $(v_i)_j$ (where $j = 1, \dots, n$), is recursively defined by

$$(4) \quad (v_i)_j = \begin{cases} \sqrt{a_i - [((v_{i-1})_i)^2 + ((v_{i-2})_i)^2]} & j = i \\ \frac{b_i - (v_{i-1})_j (v_{i-1})_{j-1}}{(v_i)_i} & j = i + 1 \\ c_i / (v_i)_i & j = i + 2 \\ 0 & \text{otherwise} \end{cases}$$

with initial conditions $v_{-1} = (a_{-1} \ 0 \ \dots \ 0)^T$ and $v_0 = (a_0 \ b_0 \ 0 \ \dots \ 0)^T$. This construction yields

$$\begin{aligned} v_1 &= \left(\sqrt{a_1 - (a_0^2 + a_{-1}^2)} \quad \frac{b_1 - b_0 a_0}{\sqrt{a_1 - (a_0^2 + a_{-1}^2)}} \quad \frac{c_1}{\sqrt{a_1 - (a_0^2 + a_{-1}^2)}} \quad 0 \quad \dots \quad 0 \right)^T \\ v_2 &= \left(0 \quad \sqrt{a_2 - \left(\frac{(b_1 - b_0 a_0)^2}{a_1 - (a_0^2 + a_{-1}^2)} + b_0^2 \right)} \quad \frac{b_2 - \frac{c_1 (b_1 - b_0 a_0)}{a_1 - (a_0^2 + a_{-1}^2)}}{\sqrt{a_2 - \left(\frac{(b_1 - b_0 a_0)^2}{a_1 - (a_0^2 + a_{-1}^2)} + b_0^2 \right)}} \quad \frac{c_2}{\sqrt{a_2 - \left(\frac{(b_1 - b_0 a_0)^2}{a_1 - (a_0^2 + a_{-1}^2)} + b_0^2 \right)}} \quad 0 \quad \dots \quad 0 \right)^T \\ &\text{etc.} \end{aligned}$$

Similar to the tridiagonal case, the constants a_{-1}, a_0 , and b_0 are taken to be non-negative numbers with the caveat that there will be some collections of initial values that will lead the decomposition to be ill-defined.

Proposition 6. *Let A be a symmetric pentadiagonal matrix. Then $A = \sum_{i=1}^n v_i v_i^T$ with v_i as defined in Equation (4). Assuming that all the components for each v_i are non-negative numbers, then A is completely positive.*

Proof. The proof is similar to tridiagonal case. Consider a symmetric pentadiagonal $n \times n$ matrix A such that the vectors in Equation (4) are well-defined. Let $V_i = v_i v_i^T$ for $i = -1, \dots, n$ and $\tilde{A} = \sum_{i=-1}^n V_i$. We wish to show that $\tilde{A} = A$. From the definition of the v_i given in Equation (4), each V_i is symmetric and pentadiagonal with only up to six nonzero entries and so \tilde{A} itself is symmetric and pentadiagonal.

Now, consider a component $\tilde{a}_{j,j+1}$ of \tilde{A} , where $j = 1, 2, \dots, n-1$. The only V_i that will have a nonzero entry in the $(j, j+1)$ -th component will be V_{j-1} and V_j as v_{j-1} and v_j are the only vectors with both the j and $(j+1)$ -th components being nonzero. The $(j, j+1)$ -th component of $V_{j-1} + V_j$ is $(v_{j-1})_j (v_{j-1})_{j+1} + (v_j)_j (v_j)_{j+1}$ which, after simplifying, is in fact b_j and so $\tilde{a}_{j,j+1} = b_j$. By symmetry, we also have $\tilde{a}_{j+1,j} = b_j$.

Now, consider a component $\tilde{a}_{j,j+2}$ of \tilde{A} , where $j = 1, 2, \dots, n-2$. The only V_i that will have a nonzero entry in the $(j, j+2)$ -th component will be V_j as v_j and v_{j+2} are the only vectors with both the j and $(j+2)$ -th components being nonzero. The value of $(v_j)_j$ is the same as the denominator of $(v_j)_{j+2}$, and so we simply obtain $\tilde{a}_{j,j+2} = c_j$. By symmetry, we also have $\tilde{a}_{j+2,j} = c_j$.

Now consider a component on the diagonal of \tilde{A} : \tilde{a}_{jj} , where $j = 1, 2, \dots, n$. The only V_i that have nonzero entries in the (j, j) -th component will be V_{j-2}, V_{j-1} , and V_j , and the sum of the respective values is precisely $\tilde{a}_{jj} = a_j$ for $j = 1, 2, \dots, n$. Therefore $A = \tilde{A} = \sum_{i=-1}^n v_i v_i^T$; i.e. A is completely positive. \square

When using Equation (4) to find a decomposition of a pentadiagonal matrix, it is simplest to choose the initial vectors v_{-1} and v_0 to both be the zero vector. However, Example 3 shows that it is sometimes necessary to choose nonzero initial conditions in order to prove that the given matrix is completely positive.

Example 3. Consider the matrix

$$A = \begin{pmatrix} 3/4 & 1/8 & 1/8 & 0 & 0 \\ 1/8 & 3/4 & 0 & 1/8 & 0 \\ 1/8 & 0 & 1/2 & 13/40 & 1/20 \\ 0 & 1/8 & 13/40 & 1/2 & 1/20 \\ 0 & 0 & 1/20 & 1/20 & 9/10 \end{pmatrix}.$$

Using Equation (4) with initial vectors v_{-1} and v_0 both taken to be the zero vector, we compute the matrix V such that $A = VV^T$ to be

$$V = \begin{pmatrix} 0 & 0 & \frac{\sqrt{3}}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{4\sqrt{3}} & \frac{\sqrt{35}}{4} & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{4\sqrt{3}} & -\frac{1}{4\sqrt{105}} & \frac{\sqrt{67}}{2} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{3}}{2} & \frac{23}{\sqrt{2345}} & \frac{\sqrt{339}}{2} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{7}}{2} & \frac{7\sqrt{3}}{2} & \sqrt{\frac{101}{113}} \end{pmatrix}.$$

We note that the component $(v_2)_3$ is negative and hence this decomposition cannot be used to prove that A is completely positive. It is not surprising that taking the initial conditions to be all zero does not work: if both v_{-1} and v_0 are zero vectors, i.e. $a_{-1} = a_0 = b_0 = 0$, then $(v_2)_3 > 0$ is equivalent to $a_1 b_2 \geq b_1 c_1$. But in A , $b_1 = c_1 = 1/8$ while $b_2 = 0$, so $a_1 b_2 < b_1 c_1$.

If we instead use the initial conditions $v_{-1} = (0 \ 0 \ \dots \ 0)^T$ and $v_0 = (\frac{1}{2} \ \frac{1}{4} \ 0 \ \dots \ 0)^T$, we obtain the decomposition $A = WW^T$, where

$$W = \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{4} & 0 & \frac{\sqrt{11}}{4} & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{4\sqrt{2}} & 0 & \frac{\sqrt{15}}{4} & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2\sqrt{11}} & \frac{13}{5\sqrt{30}} & \frac{\sqrt{4157}}{10} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{5} & \frac{23\sqrt{11}}{62355} & \sqrt{\frac{14861}{4157}} \end{pmatrix}.$$

This decomposition shows that A is in fact completely positive.

Example 4. As an analogue to Example 2 consider the matrix

$$\begin{pmatrix} 1/2 & 1/4 & 1/4 & 0 & 0 & 0 \\ 1/4 & 1/2 & 1/4 & 0 & 0 & 0 \\ 1/4 & 1/4 & 1/2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/2 & 1/2 & 0 \\ 0 & 0 & 0 & 1/2 & 1/2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

For this matrix, the construction we outline through Equation (4) will never give a well-defined decomposition regardless of the choice of initial conditions. To see why this is the case, note that $c_2 = b_3 = c_3 = 0$. Here we may assume that we have chosen initial conditions such that $(v_1)_1$, $(v_2)_2$, and $(v_3)_3$ are nonzero (otherwise the decomposition would already be ill-defined). From this we immediately obtain

$$(v_2)_4 = \frac{c_2}{(v_2)_2} = 0$$

$$(v_3)_4 = \frac{b_3 - (v_2)_4(v_2)_3}{(v_3)_3} = 0$$

$$(v_3)_5 = \frac{c_3}{(v_3)_3} = 0.$$

Therefore we can compute the following components of v_4 to be:

$$(v_4)_4 = \sqrt{a_4 - ((v_3)_4)^2 + ((v_2)_4)^2} = \sqrt{a_4} = \frac{1}{\sqrt{2}}$$

$$(v_4)_5 = \frac{b_4 - (v_3)_5(v_3)_4}{(v_4)_4} = \frac{b_4}{\sqrt{a_4}} = \frac{1}{\sqrt{2}}$$

$$(v_4)_6 = \frac{c_4}{(v_4)_4} = 0.$$

Now, all six of the components that have been calculated so far are completely independent of the initial conditions (except for the requirement that all previous components were well-defined). Therefore the vector v_5 will be independent of the initial conditions. We then find that

$$(v_5)_5 = \sqrt{a_5 - ((v_4)_5)^2 + ((v_3)_5)^2} = \sqrt{\frac{1}{2} - \left(\left(\frac{1}{\sqrt{2}} \right)^2 + 0 \right)} = 0.$$

Hence $(v_5)_6$ will not be well-defined.

Similar to Example 2, we can still make use of our construction to prove that A is completely positive by considering A as the block diagonal matrix

$$A = \begin{pmatrix} A_1 & 0_{3,2} & 0_{3,1} \\ 0_{2,3} & A_2 & 0_{2,1} \\ 0_{1,3} & 0_{1,2} & A_3 \end{pmatrix}$$

where

$$A_1 = \begin{pmatrix} 1/2 & 1/4 & 1/4 \\ 1/4 & 1/2 & 1/4 \\ 1/4 & 1/4 & 1/2 \end{pmatrix}, \quad A_2 = \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}, \quad A_3 = (1)$$

From here we can find a decomposition for the three matrices A_1 , A_2 , and A_3 separately. We find that

$$V_1 = \begin{pmatrix} 0 & 0 & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \frac{1}{2\sqrt{2}} & \frac{\sqrt{\frac{3}{2}}}{2} & 0 \\ 0 & 0 & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{6}} & \frac{1}{\sqrt{3}} \end{pmatrix}, \quad V_2 = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 \end{pmatrix}, \quad V_3 = (1)$$

where $A_1 = V_1V_1^T$, $A_2 = V_2V_2^T$, and $A_3 = V_3V_3^T$. A decomposition for A can then be formed by creating the block diagonal matrix

$$V = \begin{pmatrix} V_1 & 0_{3,3} & 0_{3,1} \\ 0_{2,5} & V_2 & 0_{2,1} \\ 0_{1,5} & 0_{1,3} & V_3 \end{pmatrix} = \begin{pmatrix} 0 & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2\sqrt{2}} & \frac{\sqrt{\frac{3}{2}}}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{6}} & \frac{1}{\sqrt{3}} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

and noting that $A = VV^T$. This proves that A is completely positive.

Similar to Example 1, we note that for any matrix M , if M has columns consisting entirely of zeros these columns can be removed from the matrix M without changing the value of MM^T . Therefore we can simplify V to be the 5×5 matrix below, rather than the 9×9 matrix above;

$$V = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 \\ \frac{1}{2\sqrt{2}} & \frac{\sqrt{\frac{3}{2}}}{2} & 0 & 0 & 0 \\ \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{6}} & \frac{1}{\sqrt{3}} & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

We leave a result analogous to Proposition 3 in the setting of symmetric pentadiagonal doubly stochastic matrices as an open problem. Example 3 shows that there is a connection between elements in A and how should one choose v_{-1} and v_0 , however it is not immediately clear in general. Consider the matrix A' which is equal to A except for the following entries:

$$\begin{aligned} a'_{11} &= a_1 - (a_0^2 + a_{-1}^2) \\ a'_{22} &= a_2 - b_0^2 \\ a'_{21} &= a'_{12} = b_1 - b_0a_0. \end{aligned}$$

Note that $A = A'$ provided the initial conditions are zero. If A' is positive definite, then all of its leading principal minors are positive. However, this does not appear to be enough to conclude that A is completely positive in this setting. Indeed, Equation (4) yields $(v_2)_3 =$

$$\frac{b_2 - \frac{c_1(b_1 - b_0a_0)}{a_1 - (a_0^2 + a_{-1}^2)}}{\sqrt{a_2 - \left(\frac{(b_1 - b_0a_0)^2}{a_1 - (a_0^2 + a_{-1}^2)} + b_0^2 \right)}}, \quad \text{and } (v_2)_3 > 0 \text{ is equivalent to } b_2 - \frac{c_1(b_1 - b_0a_0)}{a_1 - (a_0^2 + a_{-1}^2)} > 0 \text{ (assuming the}$$

denominator of $(v_2)_3$ is well-defined). This expression is equivalent to requiring that the 3×3 leading principal submatrix of A' with the last row and second last column removed, has positive determinant.

In general, requiring that $(v_i)_{i+1} > 0$, assuming the denominator is well-defined, is equivalent to requiring that the $(i+1) \times (i+1)$ leading principal submatrix of A' with the last row and second last column removed, has positive determinant.

3.3. Alternate Construction. As Example 3 illustrates, there can be some trial and error when it comes to finding a decomposition with all components being positive. Selecting initial conditions that can achieve this may be difficult or even impossible in certain cases. One workaround to this is in the case where the given matrix is block diagonal, as in Example 4.

Another technique one can use if decomposing A directly as described by Equation (2) or (4) does not yield results, is described in this Section. It can be used when the given matrix is not necessarily block diagonal. The main idea is to find matrices \tilde{A} and \hat{A} such that $A = \tilde{A} + \hat{A}$ and then decompose \tilde{A} and \hat{A} using Equation (2) or (4). If \tilde{A} and \hat{A} are completely positive with decompositions $\tilde{A} = VV^T$ and $\hat{A} = WW^T$, then A will have decomposition given by the matrix $(V \ W)$, which is simply the matrix constructed with the columns of V followed by the columns of W . Below, we provide a construction that gives A as a sum of two specified positive semidefinite matrices \tilde{A} and \hat{A} that can often be convenient to consider, but in general there are other matrices that work.

Let A be a $n \times n$ symmetric pentadiagonal doubly stochastic matrix. Recall the convention that $b_0 = b_n = c_{-1} = c_0 = c_{n-1} = c_n = 0$. Define the $n \times n$ matrix \tilde{A} to be the matrix with components $\tilde{a}_{ii} = \frac{1}{2} - b_i - b_{i-1}$ for $i \in \{1, \dots, n\}$, $\tilde{a}_{i,i+2} = \tilde{a}_{i+2,i} = c_i$, and all other components being zero. We will similarly define the $n \times n$ matrix \hat{A} to be the matrix with components $\hat{a}_{ii} = \frac{1}{2} - c_i - c_{i-2}$ for $i \in \{1, \dots, n\}$, $\hat{a}_{i,i+1} = \hat{a}_{i+1,i} = b_i$, and all other components being zero. We find that $\tilde{A} + \hat{A} = A$, as desired.

Since the property of complete positivity implies that the given matrix A is positive semidefinite, if we can find a decomposition showing that A is completely positive, it will automatically be positive semidefinite (and hence diagonally dominant by Lemma 3). If A is diagonally dominant, \tilde{A} and \hat{A} are diagonally dominant as well, and hence also positive semidefinite. As \tilde{A} and \hat{A} are much simpler than A , finding decompositions for both \tilde{A} and \hat{A} with all positive components is often much simpler (if it is possible), as the next example shows.

Example 5. Consider the matrix

$$A = \begin{pmatrix} 7/12 & 1/3 & 1/12 & 0 \\ 1/3 & 7/12 & 1/156 & 1/13 \\ 1/12 & 1/156 & 7/12 & 17/52 \\ 0 & 1/13 & 17/52 & 31/52 \end{pmatrix}.$$

Since the matrix has dimension 4 and is doubly non-negative it must be completely positive by [1]. However, if we try to decompose A using the all zero vectors as our initial conditions, we obtain

$$\begin{pmatrix} 0 & 0 & \frac{\sqrt{7}}{2} & 0 & 0 & 0 \\ 0 & 0 & \frac{2}{\sqrt{21}} & \frac{\sqrt{11}}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2\sqrt{21}} & -\frac{15}{26\sqrt{77}} & \frac{\sqrt{4217}}{26} & 0 \\ 0 & 0 & 0 & \frac{2\sqrt{7}}{13} & \frac{2491}{26\sqrt{46387}} & 4\sqrt{\frac{101}{4217}} \end{pmatrix}.$$

Note the single negative entry. We can try using different initial conditions, but taking a guess-and-check approach is not an ideal strategy. Instead, now consider the matrices \tilde{A} and \hat{A} :

$$\tilde{A} = \begin{pmatrix} 1/6 & 0 & 1/12 & 0 \\ 0 & 25/156 & 0 & 1/13 \\ 1/12 & 0 & 1/6 & 0 \\ 0 & 1/13 & 0 & 9/52 \end{pmatrix}, \quad \hat{A} = \begin{pmatrix} 5/12 & 1/3 & 0 & 0 \\ 1/3 & 11/26 & 1/156 & 0 \\ 0 & 1/156 & 5/12 & 17/52 \\ 0 & 0 & 17/52 & 11/26 \end{pmatrix}$$

Decomposing both of these we obtain

$$V = \begin{pmatrix} 0 & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{5}{2\sqrt{39}} & 0 & 0 \\ 0 & 0 & \frac{1}{2\sqrt{6}} & 0 & \frac{1}{2\sqrt{2}} & 0 \\ 0 & 0 & 0 & \frac{2\sqrt{\frac{3}{13}}}{5} & 0 & \frac{\sqrt{\frac{177}{13}}}{10} \end{pmatrix}, \quad W = \begin{pmatrix} 0 & 0 & \frac{\sqrt{\frac{5}{3}}}{2} & 0 & 0 & 0 \\ 0 & 0 & \frac{2}{\sqrt{15}} & \sqrt{\frac{61}{390}} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{\frac{5}{4758}}}{2} & \frac{5\sqrt{\frac{317}{4758}}}{2} & 0 \\ 0 & 0 & 0 & 0 & \frac{17\sqrt{\frac{183}{8242}}}{5} & \frac{2\sqrt{\frac{4286}{4121}}}{5} \end{pmatrix}$$

where $\tilde{A} = VV^T$ and $\hat{A} = WW^T$. One can check that $A = (V \ W) (V \ W)^T$, where we set $(V \ W)$ to be (we deleted unnecessary all-zero columns):

$$(5) \quad (V \ W) = \begin{pmatrix} \frac{1}{\sqrt{6}} & 0 & 0 & 0 & \frac{\sqrt{\frac{5}{3}}}{2} & 0 & 0 & 0 \\ 0 & \frac{5}{2\sqrt{39}} & 0 & 0 & \frac{2}{\sqrt{15}} & \sqrt{\frac{61}{390}} & 0 & 0 \\ \frac{1}{2\sqrt{6}} & 0 & \frac{1}{2\sqrt{2}} & 0 & 0 & \frac{\sqrt{\frac{5}{4758}}}{2} & \frac{5\sqrt{\frac{317}{4758}}}{2} & 0 \\ 0 & \frac{2\sqrt{\frac{3}{13}}}{5} & 0 & \frac{\sqrt{\frac{177}{13}}}{10} & 0 & 0 & \frac{17\sqrt{\frac{183}{8242}}}{5} & \frac{2\sqrt{\frac{4286}{4121}}}{5} \end{pmatrix}$$

This shows that A is completely positive.

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