ON THE CONSTRUCTION OF NONNEGATIVE SYMMETRIC AND NORMAL MATRICES WITH PRESCRIBED SPECTRAL DATA

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A dissertation submitted in partial fulfillment of the
requirements for the degree of

DOCTOR OF PHILOSOPHY

WASHINGTON STATE UNIVERSITY
Department of Mathematics

DECEMBER 2009

I certify that I have read this dissertation and certify that in my opinion it is fully adequate, in scope and in quality, as a dissertation for the degree of Doctor of Philosophy.

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Abstract

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Nonnegative matrices appear in many branches of mathematics, as well as in applications to other disciplines such as economics, computer science, and chemistry. Since the inception of the fundamental results by Perron and Frobenius, the area of nonnegative matrices have been a fertile field for research. In this dissertation, we consider the problem of reconstructing a nonnegative symmetric or normal matrix based on a knowledge of spectral data.

Specifically, our exposition is centered around two facets of the just-mentioned problem. First, we consider symmetric matrices with spectrum $\sigma = \{\lambda_1, \lambda_2, \ldots, \lambda_n\}$ and corresponding orthonormal set of eigenvectors $s_1, s_2, \ldots, s_n$, such that successive spectral decompositions are nonnegative:

$$\sum_{i=1}^{t} \lambda_i s_i s_i^T \geq 0, \quad t = 1, \ldots, k.$$

We determine the zero-nonzero structure of the s_i's which correspond to positive λ_i's, and provide a complete characterization of the s_i's in case the above holds for $\lambda_1 = \lambda_2 = \cdots = \lambda_t = 1$ for $t = 1, \ldots, n$. The resulting orthogonal matrices $S = [s_1, s_2, \ldots, s_n]$, which we call here extended Soules matrices, are then a generalization of the well-studied class of Soules matrices (henceforth called classical Soules matrices). Among other results,

we also prove each extended Soules matrix is the limit of a sequence of classical Soules matrices, and that the rank of symmetric matrices whose eigenvectors form an extended Soules matrix is equal to the *cp*-rank of the matrix. The other associated problem is that of characterizing the set of potential λ_i's, where $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \geq 0$, such that the above partial sum nonnegativity is accomplished for a given fixed set $s_1, s_2, \ldots, s_n$. We provide some initial results in this direction, as well as an example of how such an analysis would proceed using certain orthogonal Hadamard matrices.

Second, we consider the nonnegative (nonsymmetric) normal inverse eigenvalue problem (NNIEP), which is the problem of determining necessary and sufficient conditions on a list σ of complex numbers such that σ is the spectrum of a nonnegative normal matrix. We give a summary of some known necessary and sufficient conditions for the NNIEP, and present some preliminary results using the somewhat new technique of analyzing the eigenvectors of certain skew-symmetric matrices, and using the result to construct solution matrices for the NNIEP. Using this technique, we are able to give the strongest possible result for the NNIEP for 3×3 matrices, and make some progress on the NNIEP for 4×4 matrices. That our approach has promise is evidenced by the nonnegative normal matrix we construct whose spectrum is $\sigma = \{12\sqrt{2}, -12, 12 + i, 12 - i\}$, even though σ satisfies none of the currently known sufficient conditions for the NNIEP.

Acknowledgment

There are a multitude of people at Washington State University who have helped to shape this document, both in specific content, and in the general technical expertise its writing required. Foremost, I thank my advisor Judi McDonald, whose infinite patience, vast expertise in all things linear algebraic, and high degree of commitment my own success as a student, researcher, and teacher, has at once inspired the scope and breadth of content in this dissertation, and has challenged me to dare to reach higher. I am also very grateful to my committee members Michael Tsatsomeros and Bala Krishnamoorthy who, as excellent teachers and superb mentors, have also been essential to my graduate work and development as a mathematician.

Behind every achievement we may claim as our own, there is always a loving and supportive family, and this is especially so in my case. Without the love, support, and patience of my wife Amy, the joyous distraction of my daughter Josephine, the never-failing encouragement from my mother Lila, or the been-there-done-that, haughty expertise of my brother Brock, the first step leading to this dissertation would not have been possible.

There are also many current and former fellow graduate students at Washington State University who have been great friends, excellent colleagues, and skilled mathematicians in their own right. Specifically, I am thankful for having been considered a friend by Jong-Sam Jeon, DeAnne Morris, Amy Yielding, Liz Bodine, Jeff Douglas, and John Chuba.

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Chapter 1

Preliminaries

1.1 Introduction

Since its initial development by Perron and Frobenius at the beginning of the 20^{th} century, the theory of nonnegative matrices has progressed enormously and is currently being used and extended in such diverse fields of study as probability theory, numerical analysis, demography, economics, and dynamic programming. This scope of application is evident to anyone using the Google search engine, which utilizes nonnegative matrix theory to rank those web pages most relevant to the search terms. Some other famous examples include Leontief's input-output analysis in economics and state-transitions modeled by finite Markov chains in statistics, both of which have nonnegative matrices as primary objects of study. In all cases, an analysis of the spectrum of the underlying nonnegative matrix is of particular interest.

Often in problems of a dynamic nature, the reconstruction of a nonnegative matrix from prescribed, or desired, spectral data is essential to obtain insight into the behavior of the phenomenon being studied. This is the main theme of this dissertation, and we examine two specific facets herein. In Chapter 2, we examine nonnegative symmetric matrices for which each partial sum of its spectral decomposition expansion is also nonnegative. That is, symmetric matrices with spectrum $\sigma = \{\lambda_1, \lambda_2, \ldots, \lambda_n\}$ and orthonormal set $s_1, s_2, \ldots, s_n$ of eigenvectors, for which each partial sum of its spectral decomposition is nonnegative:

$$\sum_{i=1}^{t} \lambda_i s_i s_i^T \geq 0, \quad t = 1, \ldots, n.$$

In Section 2.2 we prove first a characterization of the sign pattern of the vectors s_i which correspond to a positive λ_i. We apply this result in Section 2.3 to the case where $\lambda_1 = \lambda_2 = \cdots = \lambda_t = 1$ for $t = 1, \ldots, n$ (which is equivalent to the above property holding for all $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \geq 0$), and obtain what we call extended Soules matrices. In turn, we show that extended Soules matrices lie in the topological closure of the set of all Soules matrices (which are now well-known), which we refer to herein as classical Soules matrices. We show also that symmetric matrices whose eigenvectors form extended Soules matrices have *cp*-rank equal to the rank, and a few other results regarding matrix functions of these symmetric matrices. In Section 2.4, we consider the problem of determining the set of λ_i's for which the above spectral decomposition property holds for a given fixed set of s_i's, and present some basic results. The solution to the problem in this case amounts to that of solving systems of linear inequalities, a process which we illustrate for certain orthogonal Hadamard matrices in 2.4.1

In Chapter 3 we explore the nonnegative inverse eigenvalue problem for normal matrices (NNIEP), which is the problem of determining necessary and sufficient conditions for a given list of complex numbers to be the spectrum of a nonnegative normal matrix. In Section 3.1, we summarize some of the necessary conditions for the general NIEP, including Karpelevich's Theorem, which outlines the solution to the stochastic NIEP (StNIEP) (the NIEP and the StNIEP are equivalent, as we outline in Section 3.1). We then very briefly summarize some sufficient conditions for the real NIEP (RNIEP) in 3.1. These conditions lead to sufficient conditions for the NNIEP, which we outline, and include a more recent result for the NIEP for circulant matrices, in Section 3.2. Prompted by the fact that the list $\sigma = \{12\sqrt{2}, -12, 12+i, 12-i\}$ does not satisfy any currently known sufficient conditions for the NNIEP, but yet is the spectrum of a nonnegative normal 4×4 matrix, a new means of examining the NNIEP, that from the perspective of eigenvectors of skew-symmetric matrices, is detailed in Section 3.3. The results obtained here lead to the strongest result available for the NNIEP in the case $n = 3$, and to some interesting preliminary results for the NNIEP in the case $n = 4$.

1.2 Standard Definitions, Notation, and Results

In this section we begin with some standard definitions, notation, and results as can be seen from any advanced text in matrix theory. Our main sources here are [13] and [25].

Denote by $M_n(S)$ the set of $n \times n$ ("square") matrices with entries from the set S; if it is not necessary to specify S, we simply write M_n and assume the entries are complex numbers. If A is a square matrix, the *spectrum* of A, denoted by $\sigma(A)$, is the set of eigenvalues of A. The *spectral radius* $\rho(A)$ of A is defined as $\rho(A) = \max\{|\lambda| : \lambda \in \sigma(A)\}$. Since we consider exclusively matrices A with real entries, any complex eigenvalues of A occur in conjugate pairs, a property we summarize by writing $\sigma(A) = \overline{\sigma(A)}$. The *trace* of A, denoted $\mathrm{tr}(A)$ is the sum of the diagonal entries of A. If $\sigma(A) = \{\lambda_1, \lambda_2, \ldots, \lambda_n\}$, it is known that $\mathrm{tr}(A) = \lambda_1 + \lambda_2 + \cdots + \lambda_n$. The set $\sigma(A)$ is the set of roots of the *characteristic polynomial*, written as a formal polynomial in t, and defined by $p_A(t) = \det(tI - A)$.

Since most of the matrices as well as the vector spaces considered in this dissertation are real, our usage of $\|\cdot\|$ with no subscript indicates the standard Euclidean norm.

If $A = [a_{ij}] \in M_n$, by $A^T = [a_{ji}] \in M_n$ we denote the *transpose* of A, and $A^* = [\bar{a}_{ji}]$

the *conjugate transpose* or *Hermitian adjoint* of A. Clearly $A^T = A^*$ if and only if $A \in M_n(\mathbb{R})$.

If $A \in M_n$ commutes with its Hermitian adjoint, i.e. $AA^* = A^*A$, A is said to be *normal*. If $A \in M_n(\mathbb{R})$ is normal, then $AA^T = A^TA$. If A is *Hermitian*, i.e. $A = A^*$, or *skew-Hermitian*, i.e. $A = -A^*$, then A is normal. Also, if $A \in M_n(\mathbb{R})$ is *symmetric*, then $A = A^T$, or skew-symmetric, then $A = -A^T$, and both symmetric and skew-symmetric matrices are also normal. Additionally, if $A \in M_n$ and $AA^* = I$, A is *unitary*, while if $A \in M_n(\mathbb{R})$ is unitary, $AA^T = I$, and A is called *orthogonal*. Both unitary and orthogonal matrices are also normal. The following result can be found in [13, Theorem 2.5.4].

Theorem 1.1 [13] *Let $A \in M_n$, with $\sigma(A) = \{\lambda_1, \lambda_2, \ldots, \lambda_n\} \subset \mathbb{C}$. The following are equivalent.*

(a) A is normal.

(b) There is an orthonormal set of n eigenvectors of A.

(c) A is unitarily diagonalizable: there is a unitary matrix U such that

$$U^*AU = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n).$$

(d) If we let $H = \frac{1}{2}(A + A^*)$ and $K = \frac{1}{2}(A - A^*)$ (H and K are Hermitian and skew-Hermitian, respectively) then $HK = KH$.

If $A \in M_n(\mathbb{R})$, we may replace "Hermitian" and "skew-Hermitian" above with "symmetric" and "skew-symmetric," but in (c) we still must in general require a unitary, rather than an orthogonal, matrix to diagonalize A. The equivalence of (a) and (c) above is known as the *Spectral Decomposition Theorem*:

Theorem 1.2 (Spectral Decomposition Theorem for Normal Matrices) *Let* $A \in M_n$, *with* $\sigma(A) = \{\lambda_1, \lambda_2, \ldots, \lambda_n\} \subset \mathbb{C}$. *Then* A *is normal if and only if there is a unitary matrix* $U = [u_1, u_2, \ldots, u_n] \in M_n$ *such that:*

$$A = \lambda_1 u_1 u_1^* + \lambda_2 u_2 u_2^* + \cdots + \lambda_n u_n u_n^* = \sum_{i=1}^{n} \lambda_i u_i u_i^*.$$

If $A \in M_n(\mathbb{R})$, we have the following result [13, Theorem 2.5.8].

Theorem 1.3 [13] *Let* $A \in M_n(\mathbb{R})$. *Then* A *is normal if and only if there is a real orthogonal matrix* $Q \in M_n(\mathbb{R})$ *such that*

$$Q^T A Q = \begin{bmatrix} A_1 & 0 & \cdots & 0 \\ 0 & A_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & A_k \end{bmatrix} \in M_n(\mathbb{R}), \quad 1 \leq k \leq n$$

where each A_j *is either a real* 1×1 *matrix or is a real* 2×2 *matrix of the form*

$$A_j = \begin{bmatrix} \alpha_j & \beta_j \\ -\beta_j & \alpha_j \end{bmatrix}.$$

If A *is symmetric, then each* A_j *is a* 1×1 *matrix, and if* A *is skew-symmetric, each* A_j *has a zero diagonal. That is, symmetric matrices have real eigenvalues, and skew-symmetric matrices have either* 0 *or purely imaginary eigenvalues.*

1.3 Nonnegative Matrices

We continue with a brief summary of terminology and fundamental results specific to nonnegative matrix theory, which we obtain largely from [1, Chapter 2], that we require herein. An $n \times n$ matrix A is said to be *reducible* if there is a permutation matrix P (a matrix with exactly one 1 in each row and 0's elsewhere) such that:

$$PAP^T = \begin{bmatrix} B & 0 \\ C & D \end{bmatrix}$$

where B and D are square matrices, or if $n = 1$ and $A = 0$. A is called *irreducible* otherwise. In this case, the spectrum $\sigma(A)$ of A is the union of the spectra of B and D. If either of B or D are reducible, we may write the matrix in lower triangular form as above, and continue the process until no more diagonal blocks are reducible, or are 1×1 nonzero matrices. Proceeding in this manner yields the *Frobenius normal form* of A:

$$QAQ^T = \begin{bmatrix} A_{11} & 0 & \cdots & 0 \\ A_{21} & A_{22} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ A_{m1} & A_{m2} & \cdots & A_{mm} \end{bmatrix}$$

for some permutation matrix Q, where the diagonal blocks A_{ii} are square and irreducible.

Irreducibility has an elegant graph-theoretic interpretation. Let $G = G(A)$ denote the *directed graph* of an $n \times n$ matrix A, which consists of n *vertices* $P_1, P_2, \ldots, P_n$ where a *directed edge* (P_i, P_j) leads from P_i to P_j if and only if $a_{ij} \neq 0$. G is said to be *strongly connected* if there is a sequence of directed edges $\{(P_i, P_{i_1}), (P_{i_1}, P_{i_2}, \ldots, (P_{i_k}, P_j))\}$ called a *path* from every vertex P_i to any other vertex P_j. If a path contains k edges, then the entry $a_{ij}^{(k)} > 0$ where $a_{ij}^{(k)}$ is the (i, j)-entry of A^k.

Theorem 1.4 [1] *Let $A \in M_n(\mathbb{R})$. The following are equivalent.*

(a) A is irreducible.

(b) The directed graph $G(A)$ is strongly connected.

(c) For each i, j there is a positive integer q such that $a_{ij}^{(q)} > 0$.

In a strongly connected graph, each vertex belongs to a *cycle*, which is a path beginning and ending at the same vertex, each edge of which is distinct. An important consequence of the above theorem is that since a strongly connected directed graph may be viewed as a union of cycles, it follows that an irreducible matrix A can be written as a sum of multiples of *cycle matrices.* If $C = [c_{ij}]$ is a cycle matrix, then C is a $\{0, 1\}$-matrix such that if $c_{ij} = 1$ then $c_{jk} = 1$ for some k, and $c_{il} = 0$ for all $l \neq j$.

A matrix $A = [a_{ij}]$ is *nonnegative* if for each i, j, $a_{ij} \geq 0$, and we write $A \geq 0$. If $A \geq 0$ and $A \neq 0$, we write $A > 0$, and if for each i, j, $a_{ij} > 0$, A is *positive*, and we write $A \gg 0$. Note that positive matrices are irreducible. We use the same terminology for vectors as well. The fundamental theorem of nonnegative matrix theory [1, Theorem 1.4] is stated (in part) as follows.

Theorem 1.5 (**Perron-Frobenius Theorem**) *Let A be an $n \times n$ irreducible nonnegative matrix. Then $\rho(A) > 0$ is an algebraically simple eigenvalue of A (i.e. it is not repeated), any other eigenvalue of A of the same modulus is also simple, and A has an entry-wise positive eigenvector corresponding to $\rho(A)$.*

Using the Frobenius normal form of a nonnegative matrix A, the Perron-Frobenius Theorem implies that the spectral radius of any square $A \geq 0$ is an eigenvalue, which corresponds to a nonnegative eigenvector.

We remark that the full statement of the theorem naturally includes the case in which A is reducible and $\sigma(A)$ contains h eigenvalues λ_i such that $\rho(A) = |\lambda_i|$ for $i = 1, \ldots, h$. Such a matrix is said to be *cyclic of index h*. In this thesis, the nonnegative matrices under consideration are assumed to be either irreducible, or cyclic of index 1, unless otherwise noted.

Chapter 2

On a Spectral Decomposition Property of Nonnegative Symmetric Matrices

According to the Spectral Decomposition Theorem, if $A \in M_n(\mathbb{R})$ is symmetric with spectrum $\sigma(A) = \{\lambda_1, \lambda_2, \dots, \lambda_n\} \subset \mathbb{R}$, $\Lambda = \operatorname{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$, and $R = [r_1, r_2, \dots, r_n]$ is an orthogonal matrix such that $Ar_i = \lambda_i r_i$, then $A = R\Lambda R^T$, hence:

$$A = \lambda_1 r_1 r_1^T + \lambda_2 r_2 r_2^T + \cdots + \lambda_n r_n r_n^T = \sum_{i=1}^{n} \lambda_i r_i r_i^T. \tag{2.1}$$

The principal aim of this chapter is to analyze spectral decompositions of the form (2.1) for nonnegative symmetric matrices which satisfy the additional caveat that the λ_i's are nonnegative and ordered non-increasingly, and each partial sum in (2.1) is nonnegative. That is, let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \geq 0$ and consider the following sequence:

$$\sum_{i=1}^{t} \lambda_i r_i r_i^T \geq 0, \;\; t = 1, \dots, n. \tag{2.2}$$

The purpose of this chapter is to examine the following two problems which arise in consideration of (2.2): (1) fix the λ_i's and analyze the structure of orthogonal matrices R satisfying (2.2), and (2) fix R and analyze the set of n-tuples $(\lambda_1, \lambda_2, \dots, \lambda_t, 0, \dots, 0) \in \mathbb{R}^n$ for $t = 1, \dots, n$.

This chapter is organized as follows. In Section 2.1, we introduce the definitions and notation used throughout the chapter, and in Section 2.2, we begin with our main result (Theorem 2.1) characterizing those orthogonal matrices satisfying (2.2) with the

λ_i's subject to more general conditions. Section 2.3 concerns problem (1) where each $\lambda_i = 1$, and we call the resulting matrices *extended Soules matrices*; in subsections 2.3.1 and 2.3.2, we examine further properties of extended Soules matrices as they relate to matrix functions and completely positive matrices. In Section 2.4, we investigate problem (2) by utilizing specific examples of orthogonal matrices. Finally, in Section 2.5 we summarize our results, and describe open problems.

2.1 Some Additional Definitions and Notation

In this section we summarize the main body of terminology employed in this chapter. If $A > 0$ or $A < 0$, we say A is *mono-signed*, and if $A \gg 0$ or $A \ll 0$, A is *strictly mono-signed*. If A contains both positive and negative entries, we say A is *multi-signed*. We will also use these definitions for vectors x in $\mathbb{R}^n$.

The *support* of the matrix A is the set $\{(i,j) : a_{i,j} \neq 0\}$, and the *support* of the vector x is $\{i : x_i \neq 0\}$, which we will denote by $\mathrm{supp}(A)$ and $\mathrm{supp}(x)$, respectively. The *positive support* of the matrix A, denoted $\mathrm{supp}_+(A)$ is the set $\{(i,j) : a_{i,j} > 0\}$, and the *negative support* of A, denoted $\mathrm{supp}_-(A)$, is $\{(i,j) : a_{i,j} < 0\}$.

If two matrices or vectors of the same size have disjoint supports, we say they have *non-overlapping support*; otherwise they have *overlapping support*. Given two matrices X and Y of the same size with overlapping supports, if the support of X is contained in that of Y we say that X has *completely overlapping support* with Y, or that the support of X *completely overlaps* the support of Y.

A *partition of* n is a partition of the set $\langle n\rangle = \{1, 2, \ldots, n\}$ into pairwise disjoint subsets whose union is $\langle n\rangle$. Specifically, an *m-partition of* n is a partition of $\langle n\rangle$ into

m disjoint subsets. We assume that the elements within each subset of a partition are arranged in increasing order. If $A \in M_n$ and $\mathscr{R}$, $\mathscr{C}$ are p- and q-partitions of n, respectively, the matrix $A[\mathscr{R}_i|\mathscr{C}_j]$ is the submatrix of A whose rows are indexed by the elements $\mathscr{R}_i$ and columns indexed by $\mathscr{C}_j$ of the partitions. Finally, if $\mathscr{N} \subset \langle n \rangle$, we write

$$x_{\mathscr{N}} = \begin{cases} x_i & i \in \mathscr{N}, \\ 0 & i \notin \mathscr{N}. \end{cases}$$

2.2 Main Theorem

In this section we state and prove the main theorem of this chapter. Let $S \in M_n(\mathbb{R})$ be an orthogonal matrix with $S = [s_1, s_2, \ldots, s_n]$ and $\sigma = \{\lambda_1, \lambda_2, \ldots, \lambda_n\}$ an arbitrary (not necessarily ordered) sequence of real numbers. If

$$\sum_{i=1}^{t} \lambda_i s_i s_i^T \geq 0, \ t = 1, \ldots, n, \tag{2.3}$$

we say *the pair* (S, σ) *satisfies* (2.3). We now prove that the structure of the matrix S satisfying (2.3) for some sequence σ can be completely characterized.

Theorem 2.1 *Let $S = [s_1, \ldots, s_n]$ be an orthogonal matrix and $\sigma = \{\lambda_1, \lambda_2, \ldots, \lambda_n\}$ a sequence of real numbers with exactly p nonzero elements. That is, $\lambda_{i_1}, \lambda_{i_2}, \ldots, \lambda_{i_p}$ are nonzero, where $i_1 < i_2 < \cdots < i_p$. If the pair (S, σ) satisfies (2.3), then s_{i_1} is mono-signed, $\lambda_{i_1} > 0$, and for each $2 \leq j \leq p$, s_{i_j} is either*

(i) mono-signed and has non-overlapping support with each of $s_{i_1}, \ldots, s_{i_{j-1}}$; or

(ii) multi-signed and has completely overlapping support with exactly one mono-signed s_{i_k} with $k < j$.

Moreover, for each mono-signed s_{i_j}, we require $\lambda_{i_j} > 0$.

Conversely, if s_{i_1} *is mono-signed and for each* $2 \leq j \leq p$, s_{i_j} *satisfies either (i) or (ii) then there exists a sequence* σ *whose nonzero elements are* $\lambda_{i_1}, \lambda_{i_2}, \ldots, \lambda_{i_p}$, *where* $\lambda_{i_j} > 0$ *if* s_{i_j} *is mono-signed, such that the pair* (S, σ) *satisfies* (2.3).

Proof. For convenience of notation, assume the first p entries of σ are nonzero.

Since (2.3) is invariant under row permutation, we write s_1 as follows:

$$s_1 = \begin{bmatrix} s_{1,1} \\ 0 \end{bmatrix},$$

where $s_{1,1}$ is strictly mono-signed. Partition s_2 conformally:

$$s_2 = \begin{bmatrix} s_{2,1} \\ s_{2,2} \end{bmatrix}.$$

Suppose s_2 satisfies the following:

$$s_2^T s_1 = s_{1,1}^T s_{2,1} = 0, \tag{2.4a}$$

$$\lambda_1 s_1 s_1^T + \lambda_2 s_2 s_2^T = \begin{bmatrix} \lambda_1 s_{1,1} s_{1,1}^T + \lambda_2 s_{2,1} s_{2,1}^T & \lambda_2 s_{2,1} s_{2,2}^T \\ \lambda_2 s_{2,2} s_{2,1}^T & \lambda_2 s_{2,2} s_{2,2}^T \end{bmatrix} \geq 0. \tag{2.4b}$$

By (2.4a), $s_{2,1}$ is either multi-signed or 0, and considering the $(2,2)$ block of (2.4b), $s_{2,2}$ is either 0 or mono-signed, and in the latter case, we also require $\lambda_2 > 0$. Nonnegativity of the off-diagonal blocks of (2.4b) implies either that if $s_{2,2}$ is mono-signed then $s_{2,1} = 0$ and if $s_{2,1}$ is multi-signed then $s_{2,2} = 0$. Hence, s_2 satisfies either (i) or (ii) above.

Proceeding by induction, assume s_i satisfies either (i) or (ii) for $i = 1, \ldots, k$ $(k < p)$. Suppose m of the s_i's satisfy (i), and denote them by $s_1 = s_{c_1}, s_{c_2}, \ldots, s_{c_m}$ with $c_{l-1} < c_l$, and also that $\lambda_{c_l} > 0$ for each $l = 1, \ldots, m$. The induction hypothesis and the invariance of (2.3) under row permutation allow us to partition these vectors as follows:

$$s_1 = \begin{bmatrix} s_{1,1} \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix}, s_{c_2} = \begin{bmatrix} 0 \\ s_{c_2,2} \\ \vdots \\ 0 \\ 0 \end{bmatrix}, \ldots, s_{c_m} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ s_{c_m,m} \\ 0 \end{bmatrix}. \tag{2.5}$$

We also assume each of the $s_1, \ldots, s_k$ are partitioned in this manner, and we write:

$$\sum_{i=1}^{k} \lambda_i s_i s_i^T = \begin{bmatrix} S_1 & 0 & \cdots & 0 & 0 \\ 0 & S_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & S_m & 0 \\ 0 & 0 & \cdots & 0 & 0 \end{bmatrix}, \tag{2.6}$$

where $S_i \geq 0$ for each i. Partition s_{k+1} as follows:

$$s_{k+1} = \begin{bmatrix} s_{k+1,1} \\ s_{k+1,2} \\ \vdots \\ s_{k+1,m} \\ s_{k+1,m+1} \end{bmatrix}. \tag{2.7}$$

Let s_{k+1} satisfy the following:

$$s_{k+1}^T s_{c_l} = s_{k+1,l}^T s_{c_l,l} = 0 \text{ for each } l = 1, \ldots, m, \tag{2.8a}$$

$$\sum_{i=1}^{k+1} \lambda_i s_i s_i^T =$$

$$\begin{bmatrix} S_1 + \lambda_{k+1} s_{k+1,1} s_{k+1,1}^T & \cdots & \lambda_{k+1} s_{k+1,1} s_{k+1,m}^T & \lambda_{k+1} s_{k+1,1} s_{k+1,m+1}^T \\ \vdots & \ddots & \vdots & \vdots \\ \lambda_{k+1} s_{k+1,m} s_{k+1,1}^T & \cdots & S_m + \lambda_{k+1} s_{k+1,m} s_{k+1,m}^T & \lambda_{k+1} s_{k+1,m} s_{k+1,m+1}^T \\ \lambda_{k+1} s_{k+1,m+1} s_{k+1,1}^T & \cdots & \lambda_{k+1} s_{k+1,m+1} s_{k+1,m}^T & \lambda_{k+1} s_{k+1,m+1} s_{k+1,m+1}^T \end{bmatrix} \geq 0. \tag{2.8b}$$

Since each of the $s_{c_l,l}$'s are mono-signed, it follows from (2.8a) that each of the $s_{k+1,l}$'s are multi-signed or 0. As before, the $(m+1, m+1)$ block of (2.8b) implies $s_{k+1,m+1}$ is either 0 or mono-signed, with the latter case implying $\lambda_{k+1} > 0$. The off-diagonal blocks of (2.8b) thus yield that if $s_{k+1,m+1}$ is mono-signed, then the $s_{k+1,l}$'s are all 0, and if any of the $s_{k+1,l}$'s are multi-signed, then $s_{k+1,q} = 0$ for each $q \neq l$. That is, s_{k+1} satisfies (i) or (ii) above. This completes the induction, and the proof of the first part.

To prove the converse, we shall continue to assume the first p columns of S satisfy (i) or (ii) above, with s_1 mono-signed. Let $\lambda_1 = 1$, since $s_1 s_1^T \geq 0$. As before, we write s_1 as follows:

$$s_1 = \begin{bmatrix} s_{1,1} \\ 0 \end{bmatrix},$$

where $s_{1,1}$ is strictly mono-signed, and partition s_2 conformally:

$$s_2 = \begin{bmatrix} s_{2,1} \\ s_{2,2} \end{bmatrix}.$$

Note that it follows from (i) and (ii) that $s_{2,1}s_{2,2}^T = 0$ and $s_{2,2}s_{2,1}^T = 0$, hence we compute:

$$s_1 s_1^T + \lambda_2 s_2 s_2^T = \begin{bmatrix} s_{1,1}s_{1,1}^T + \lambda_2 s_{2,1}s_{2,1}^T & 0 \\ 0 & \lambda_2 s_{2,2}s_{2,2}^T \end{bmatrix}. \tag{2.9}$$

If s_2 satisfies (i), $s_{2,1} = 0$ and $s_{2,2}$ is mono-signed, hence $s_{2,1}s_{2,1}^T = 0$ and we may take $\lambda_2 = 1$. Otherwise, if s_2 satisfies (ii), then $s_{2,2} = 0$, so $s_{2,2}s_{2,2}^T = 0$, and $s_{2,1}$ is multi-signed. To analyze this case more concisely requires additional notation. Let $A = [a_{i,j}] \in M_n(\mathbb{R})$ and $B = [b_{i,j}] \in M_n(\mathbb{R})$, where B has at least one positive and one negative entry. Define the functions $l(\cdot,\cdot)$ and $L(\cdot,\cdot)$ as follows:

$$l(A,B) = \max_{(i,j)\in \text{supp}_+(B)} \left\{ \frac{-a_{i,j}}{b_{i,j}} \right\},$$

$$L(A,B) = \min_{(i,j)\in \text{supp}_-(B)} \left\{ \frac{a_{i,j}}{|b_{i,j}|} \right\}.$$

A crucial observation with respect to our assumption is that if $A \geq 0$, B is multi-signed, and the support of A completely overlaps the support of B, then $l(A,B) < 0 < L(A,B)$. Accordingly, putting $l_2 = l(s_1 s_1^T, s_2 s_2^T)$ and $L_2 = L(s_1 s_1^T, s_2 s_2^T)$, we clearly have $s_1 s_1^T + \lambda_2 s_2 s_2^T \geq 0$ if $l_2 \leq \lambda_2 \leq L_2$, and $L_2 > 0$. Hence, if s_2 satisfies (i) or (ii), we select λ_2 as follows:

$$\lambda_2 = \begin{cases} 1 & \text{if } s_2 \text{ satisfies } (i), \\ L_2 & \text{if } s_2 \text{ satisfies } (ii). \end{cases}$$

We now proceed by induction, assuming s_i satisfies either (i) or (ii) for $i = 1,\ldots,k$ ($k < p$). Suppose m of the s_i's satisfy (i), and denote them by $s_1 = s_{c_1}, s_{c_2}, \ldots, s_{c_m}$ with $c_{q-1} < c_q$. We also assume $\lambda_j \neq 0$ for $j = 1,\ldots,k$, and also that $\lambda_{c_q} > 0$ for each $q = 1,\ldots,m$ (we may take each to be 1). Partition the s_{c_q}'s as in (2.5), where we assume also that $s_1,\ldots,s_k$ are partitioned in the same manner. We may also write $\sum_{i=1}^k \lambda_i s_i s_i^T$

as in (2.6) where, again, each $S_i \geq 0$, and partition s_{k+1} conformably with the previous s_j's as in (2.7). Then, applying our assumptions as in (2.9), we have:

$$\sum_{i=1}^{k+1} \lambda_i s_i s_i^T =$$

$$\begin{bmatrix} S_1 + \lambda_{k+1} s_{k+1,1} s_{k+1,1}^T & \cdots & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & S_m + \lambda_{k+1} s_{k+1,m} s_{k+1,m}^T & 0 \\ 0 & \cdots & 0 & \lambda_{k+1} s_{k+1,m+1} s_{k+1,m+1}^T \end{bmatrix}. \quad (2.10)$$

Thus if s_{k+1} satisfies (i), then $s_{k+1,j} = 0$ for $j = 1, \ldots, m$, hence we may select $\lambda_{k+1} = 1$. If s_{k+1} satisfies (ii), then $s_{k+1,m+1} = 0$ and each of the $s_{k+1,j}$'s is either multi-signed or 0 for $j = 1, \ldots, m$. Moreover, the support of $\sum_{i=1}^{k} \lambda_i s_i s_i^T$ completely overlaps the support of s_{k+1}. Define:

$$l_{k+1} = l\left(\sum_{i=1}^{k} \lambda_i s_i s_i^T, s_{k+1} s_{k+1}^T\right) \quad \text{and} \quad L_{k+1} = L\left(\sum_{i=1}^{k} \lambda_i s_i s_i^T, s_{k+1} s_{k+1}^T\right).$$

Then (2.10) is nonnegative if $l_{k+1} \leq \lambda_{k+1} \leq L_{k+1}$, and $L_{k+1} > 0$. So, if s_{k+1} satisfies (i) or (ii), we may select λ_{k+1} as follows:

$$\lambda_{k+1} = \begin{cases} 1 & \text{if } s_{k+1} \text{ satisfies (i),} \\ L_{k+1} & \text{if } s_{k+1} \text{ satisfies (ii).} \end{cases}$$

This completes the induction and ends the proof. $\square$

Although the more general problem of analyzing pairs (S, σ) with σ not subject to any particular ordering conditions is interesting and theoretically sophisticated, we do not treat this problem here. In the next section we apply the forward direction of Theorem 2.1 to the case where each $\lambda_i = 1$, and in the following section we (partially) apply the opposite direction to the case in which $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \geq 0$.

2.3 Extended Soules Matrices

Let $S = [s_1, \ldots, s_n] \in M_n$ be an orthogonal matrix whose columns satisfy the following property:

$$\sum_{i=1}^{t} s_i s_i^T \geq 0 \quad t = 1, \ldots, n. \tag{2.11}$$

Clearly s_1 is mono-signed. We call S an *extended Soules matrix*, and if, in addition, s_1 strictly mono-signed, we call S a *classical Soules matrix*.

Our first result is a generalization of [10, Observation 2.1] that was proved for classical Soules matrices only (although the proof, which we include for completeness, is the same) and that specifies the connection between (2.11) and (2.2). In particular, it indicates that (2.11) holding with s_1 mono-signed is equivalent to (2.2) holding *for all* sequences $\sigma = \{\lambda_1, \lambda_2, \ldots, \lambda_n\}$ with $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \geq 0$.

Theorem 2.2 *Let $S = [s_1, \cdots s_n] \in M_n$ be orthogonal and s_1 be mono-signed. Then*

$$\sum_{i=1}^{t} s_i s_i^T \geq 0 \quad t = 1, \ldots, n,$$

i.e. S is an extended Soules matrix, if and only if

$$\sum_{i=1}^{t} \lambda_i s_i s_i^T \geq 0, \ t = 1, \ldots, n,$$

for every sequence $\sigma = \{\lambda_1, \lambda_2, \ldots, \lambda_n\}$ with $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \geq 0$.

Proof. Sufficiency of the latter condition follows by taking $\lambda_1 = \lambda_2 = \cdots = \lambda_n = 1$, so we need only prove it is necessary. Toward this end, for each $1 \leq j \leq n$, define $\Lambda_j = \text{diag}(1, \ldots, 1, 0, \ldots, 0)$, where the first j diagonal entries of Λ_j are equal to 1, and all other entries are 0. If $\Lambda = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$ with $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \geq 0$, observe that we may rewrite Λ as follows:

$$\Lambda = (\lambda_1 - \lambda_2)\Lambda_1 + (\lambda_2 - \lambda_3)\Lambda_2 + \cdots + (\lambda_{n-1} - \lambda_n)\Lambda_{n-1} + \lambda_n \Lambda_n.$$

Notice that:

$$\sum_{i=1}^{t} s_i s_i^T = S\Lambda_t S^T \geq 0 \quad t = 1, \ldots, n$$

hence we have:

$$\sum_{i=1}^{t} \lambda_i s_i s_i^T = (\lambda_1 - \lambda_2) S\Lambda_1 S^T + \cdots + (\lambda_{t-1} - \lambda_t) S\Lambda_{t-1} S^T + \lambda_t S\Lambda_t S^T \geq 0$$

for $t = 1, \ldots, n$. Since $\sigma = \{\lambda_1, \lambda_2, \ldots, \lambda_n\}$ is an arbitrary sequence satisfying $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \geq 0$, the result follows. $\square$

Remark 2.3 If S is a classical Soules matrix, it is shown in [10, Theorem 2.2] that, associated with S, there is a sequence $\mathscr{N}_1, \ldots, \mathscr{N}_i$, $i = 1, \ldots, n$ of partitions of n, with $\mathscr{N}_1 = \{\mathscr{N}_{1,1}\}, \ldots, \mathscr{N}_i = \{\mathscr{N}_{i,1}, \ldots, \mathscr{N}_{i,i}\}$, where $\mathscr{N}_{1,1} = \langle n \rangle$ and $\mathscr{N}_i$ is constructed from $\mathscr{N}_{i-1}$ by partitioning exactly one of the sets $\mathscr{N}_{i-1,j}$ into two subsets $\mathscr{N}_{i,j}$, $\mathscr{N}_{i,j+1}$, while leaving the remaining sets intact. Letting $s_1 = s$ and $s_{\mathscr{N}_{i,j}} = s^{(i,j)}$, the just-mentioned sequence determines $s_2, \ldots, s_n$ (up to a factor of ± 1) in terms of s in the following way:

$$s_i = \frac{1}{\sqrt{\|s^{(i,j)}\|^2 + \|s^{(i,j+1)}\|^2}} \left(\frac{\|s^{(i,j+1)}\|}{\|s^{(i,j)}\|} s^{(i,j)} - \frac{\|s^{(i,j)}\|}{\|s^{(i,j+1)}\|} s^{(i,j+1)} \right), \quad i \geq 2. \qquad (2.12)$$

Finally, we note that in [34], Stuart describes an algorithm based on inflation matrices which can be used as an alternative to (2.12) to determine whether a matrix is Soules.

Observe that any convergent sequence of orthogonal matrices satisfying (2.3) has an orthogonal limit which also satisfies (2.3). Consequently, the closure of the (open) set of classical Soules matrices is contained in the set of extended Soules matrices. In order to show that inclusion holds also, we shall first describe the structure of extended Soules matrices. As a first step, we state the following lemma, which is actually a corollary of the forward direction of Theorem 2.1.

Lemma 2.4 *Let $S = [s_1, \ldots, s_n]$ be an extended Soules matrix. Then s_1 is mono-signed, and for each $i \geq 2$, s_i is either*

(i) mono-signed and has non-overlapping support with each of $s_1, \ldots, s_{i-1}$.

(ii) multi-signed and has overlapping support with exactly one mono-signed s_j with $j < i$.

Proof. Take $\lambda_1 = \lambda_2 = \cdots = \lambda_n = 1$ in the forward direction of Theorem 2.1. $\square$

The converse of Lemma 2.4 is false, as the following example shows.

Example 2.5 *Consider the following two matrices:*

$$A = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & -\frac{1}{\sqrt{2}} & 0 \\ \frac{1}{2} & -\frac{1}{2} & 0 & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{2} & -\frac{1}{2} & 0 & 0 & -\frac{1}{\sqrt{2}} \end{bmatrix}, \quad B = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 \\ \frac{1}{2} & \frac{1}{\sqrt{2}} & 0 & \frac{1}{2} & 0 \\ \frac{1}{2} & -\frac{1}{\sqrt{2}} & 0 & \frac{1}{2} & 0 \\ \frac{1}{2} & 0 & 0 & -\frac{1}{2} & \frac{1}{\sqrt{2}} \\ \frac{1}{2} & 0 & 0 & -\frac{1}{2} & -\frac{1}{\sqrt{2}} \end{bmatrix}.$$

Both matrices satisfy the conclusion of Lemma 2.4. However, A is an extended Soules matrix, and the matrix B, which may be obtained from A by interchanging columns 2 and 4, is not. In particular, (2.11) *is invariant only under certain column permutations.*

With Lemma 2.4 in hand, we have the following complete characterization of extended Soules matrices.

Theorem 2.6 *If $S = [s_1, \ldots, s_n]$ is an extended Soules matrix, then there exist m-partitions $\{\mathscr{R}_1, \ldots, \mathscr{R}_m\}$ and $\{\mathscr{C}_1, \ldots, \mathscr{C}_m\}$ of n, where $\mathscr{R}_i$ and $\mathscr{C}_i$ have the same cardinality, such that $S[\mathscr{R}_i|\mathscr{C}_j] = 0$ if $i \neq j$, and $S[\mathscr{R}_i|\mathscr{C}_i]$ is a classical Soules matrix for each $i = 1, \ldots, m$.*

Conversely, if $S_1, \ldots, S_m$ are classical Soules matrices whose orders sum to n, then for any m-partitions $\{\mathscr{R}_1, \ldots, \mathscr{R}_m\}$ and $\{\mathscr{C}_1, \ldots, \mathscr{C}_m\}$ of n such that $\mathscr{R}_i$ and $\mathscr{C}_i$ have the same cardinality as the order of S_i, the matrix S such that $S[\mathscr{R}_i|\mathscr{C}_j] = 0$ if $i \neq j$, and $S[\mathscr{R}_i|\mathscr{C}_i] = S_i$ for $i = 1, \ldots, m$, is an extended Soules matrix.

Proof. If $S = [s_1, \ldots, s_n]$ is an extended Soules matrix, by Lemma 2.4 there exists a positive integer $m \leq n$ such that the columns $s_1 = s_{c_1}, s_{c_2}, \ldots, s_{c_m}$ are mono-signed. Let r_i be the cardinality of the set $\operatorname{supp}(s_{c_i})$, and define m-partitions $\{\mathscr{R}_1, \ldots, \mathscr{R}_m\}$ and $\{\mathscr{C}_1, \ldots, \mathscr{C}_m\}$ of n as follows: for each $i = 1, \ldots, m$,

$$\mathscr{R}_i = \operatorname{supp}(s_{c_i}) \quad \text{and} \quad \mathscr{C}_i = \{c_i = c_{i,1}, c_{i,2}, \ldots, c_{i,r_i}\}, \tag{2.13}$$

where the $c_{i,j}$'s refer to those columns $s_{c_{i,j}}$ which, by Lemma 2.4, are multi-signed (for $j = 2, \ldots, r_i$) and have overlapping support with s_{c_i}. Since every other column of S has non-overlapping support with the columns indexed by $\mathscr{C}_i$, it follows not only that $S[\mathscr{R}_i|\mathscr{C}_j] = 0$ if $i \neq j$, but also $S[\mathscr{R}_i|\mathscr{C}_i]$ has a strictly mono-signed first column and satisfies (2.11). Hence $S[\mathscr{R}_i|\mathscr{C}_i]$ is a classical Soules matrix. Since this holds for each $i = 1, \ldots, m$, the result follows.

The converse follows easily, since the hypothesis guarantees (2.11) is satisfied for each pair of m-partitions with the given property. Note that our assumption that the elements of each $\mathscr{C}_i$ are listed in increasing order is critical here. $\square$

Remark 2.7 If each set in $\mathscr{R}$ is composed of consecutive integers, then the mono-signed columns of S have the form (2.7), hence each summand in (2.11) has the form (2.6). In this case, (2.11) is a direct sum for each t. If, in addition, the same is true for the sets in $\mathscr{C}$, then $\mathscr{R} = \mathscr{C}$, and the resulting extended Soules matrix is a direct sum of classical Soules matrices. This is formally proved in Section 2.3.2 as Corollary 2.14(i) to Theorem 2.6.

Remark 2.8 Let $n_1, \ldots, n_m$ be positive integers such that $n_1 + \cdots + n_m = n$, and define:

$$r_0 = 0 \quad \text{and} \quad r_i = \sum_{j=1}^{i} n_i.$$

If S is an extended Soules matrix such that $\mathscr{R}$ and $\mathscr{C}$ are m-partitions of n as in Theorem 2.6 such that:

$$\mathscr{R}_i = \{r_{i-1}+1, \ldots, r_i\} \quad \text{and} \quad \mathscr{C}_i = \{i, m-i-2+r_{i-1}, \ldots, m-i+r_i\},$$

then S has the following form:

$$\begin{bmatrix} s_{1,1} & \cdots & 0 & S[\mathscr{R}_1'|\mathscr{C}_1'] & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & s_{m,1} & 0 & \cdots & S[\mathscr{R}_m'|\mathscr{C}_m'] \end{bmatrix}, \tag{2.14}$$

where the $s_{i,1}$'s are strictly mono-signed,

$$\mathscr{R}_i' = \mathscr{R}_i \setminus \{r_{i-1}+1\} \quad \text{and} \quad \mathscr{C}_i' = \mathscr{C}_i \setminus \{i\},$$

and for each $i = 1, \ldots, m$, the $(n_i - 1) \times n_i$ matrix $S[\mathscr{R}_i'|\mathscr{C}_i']$ has multi-signed columns. Specifically, for every extended Soules matrix S there are permutation matrices P and Q such that PSQ has the form (2.14).

Now, let $\mathbb{S}_n$ and $\mathbb{G}_n$ denote the set of all $n \times n$ classical and extended Soules matrices, respectively. Using the form (2.14), we will now prove that every extended Soules matrix is the limit of a sequence of classical Soules matrices.

Theorem 2.9 *The closure* $\overline{\mathbb{S}}_n$ *of* $\mathbb{S}_n$ *coincides with* $\mathbb{G}_n$*, i.e.* $\overline{\mathbb{S}}_n = \mathbb{G}_n$.

Proof. Clearly $\mathbb{S}_n \subset \mathbb{G}_n$; that $\overline{\mathbb{S}}_n \subseteq \mathbb{G}_n$ follows from the fact that orthogonality and (2.11) hold for the limit of any convergent sequence of classical Soules matrices. We need only show that every extended Soules matrix S is the limit of a sequence of classical Soules matrices. In view of Remark 2.8, it suffices to show this for S of the form (2.14). Accordingly, let $\epsilon \in (0,1)$ and define:

$$s_1^{(\epsilon)} = \sqrt{\frac{1-\epsilon}{1-\epsilon^m}} \begin{bmatrix} |s_{1,1}| \\ |s_{2,1}|\sqrt{\epsilon} \\ \vdots \\ |s_{m,1}|\sqrt{\epsilon^{m-1}} \end{bmatrix},$$

where, for definiteness, we assume $s_{1,1} \gg 0$. For $j = 2, \ldots, m$, let $s_j^{(\epsilon)}$ be partitioned conformably with $s_1^{(\epsilon)}$ where:

$$s_j^{(\epsilon)} = \frac{\operatorname{sgn}(s_{j,1})(1-\epsilon)}{\sqrt{(1-\epsilon^{m-j+2})(1-\epsilon^{m-j+1})}} \begin{bmatrix} 0 \\ \vdots \\ 0 \\ -|s_{j-1,1}|(1-\epsilon^{m-j+1})\sqrt{\epsilon} \\ |s_{j,1}| \\ |s_{j+1,1}|\sqrt{\epsilon} \\ \vdots \\ |s_{m,1}|\sqrt{\epsilon^{m-j}} \end{bmatrix}.$$

Finally, in view of Remark 2.3 and (2.12), we define:

$$[s_{m+1}^{(\epsilon)}, \ldots, s_n^{(\epsilon)}] = \begin{bmatrix} S[\mathscr{R}_1'|\mathscr{C}_1'] & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & S[\mathscr{R}_m'|\mathscr{C}_m'] \end{bmatrix},$$

for $\mathscr{R}_i'$, $\mathscr{C}_i'$ as defined in Remark 2.8. It is easily checked that the matrix $S^{(\epsilon)} = [s_1^{(\epsilon)}, \ldots, s_n^{(\epsilon)}]$ is a classical Soules matrix for every $\epsilon \in (0,1)$, and since $S^\epsilon \to S$ as $\epsilon \to 0^+$, the proof is complete. □

2.3.1 On Matrix Functions and Exponentially Nonnegativity

In this section we describe a few results regarding matrix functions of diagonalizable matrices that are diagonalized by extended Soules matrices. Our attention here will be confined to monotonic real functions defined on $\mathbb{R}$.

Theorem 2.10 *Let S be an orthogonal matrix, and f a nondecreasing function mapping $\mathbb{R}$ onto $(0,\infty)$. Then $f(S\Lambda S^T)$ is nonnegative for all diagonal matrices Λ with non-increasing diagonal entries if and only if S is an extended Soules matrix.*

Proof. Note that $f(S\Lambda S^T) = Sf(\Lambda)S^T = S \cdot \mathrm{diag}\{f(\lambda_1), \ldots, f(\lambda_n)\} \cdot S^T$, and also that the assumptions on f imply that there is a decreasing sequence $\{x_k\}$ such that $f(x_k) = 1/k$ for $k = 1, 2, \ldots$. Let $f(S\Lambda S^T) \geq 0$ for all $\Lambda = \mathrm{diag}\{\lambda_1, \ldots, \lambda_n\}$ where $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. For each $t = 1, \ldots, n$ and positive integer k define:

$$\Lambda_k^{(t)} = \mathrm{diag}\{\underbrace{x_1, \ldots, x_1}_{\text{t terms}}, x_k, \ldots, x_k\}.$$

Then, it follows that

$$f(S\Lambda_k^{(t)}S^T) = \sum_{i=1}^{t} s_i s_i^T + \frac{1}{k}\sum_{i=t}^{n} s_i s_i^T \geq 0$$

for all $k = 1, 2, \ldots$. Letting $k \to \infty$ for each $t = 1, \ldots, n$ yields (2.11), hence S is an extended Soules matrix.

Conversely, suppose S is an extended Soules matrix, and let $\Lambda = \mathrm{diag}\{\lambda_1, \ldots, \lambda_n\}$ with $\lambda_1 \geq \cdots \geq \lambda_n$. Note that $f(S\Lambda S^T)$ may be written as follows:

$$f(S\Lambda S^T) = \sum_{t=1}^{n-1}(f(\lambda_t) - f(\lambda_{t+1}))\sum_{i=1}^{t} s_i s_i^T + f(\lambda_n)I.$$

Hence, it follows from (2.11) and our assumptions on f that $f(S\Lambda S^T) \geq 0$ for all diagonal matrices Λ with non-increasing diagonal entries. □

One direction of the following immediate corollary of Theorem 2.10 appeared in [10, Lemma 2.3] (under a slightly stronger hypothesis). Since the same proof still applies under our more general assumptions, we include it for completeness.

Corollary 2.11 *Let S be an orthogonal matrix, and g a non-increasing function mapping $(0, \infty)$ onto itself. Then $g(S\Lambda S^T)$ is a nonsingular M-matrix for every nonnegative diagonal matrix Λ with positive, non-increasing diagonal entries if and only if S is an extended Soules matrix.*

Proof. First we make some preliminary observations. If $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$, then:

$$g(S\Lambda S^T) = Sg(\Lambda)S^T = S \cdot \mathrm{diag}(g(\lambda_1), g(\lambda_2), \ldots, g(\lambda_n)) \cdot S^T.$$

Also, if $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n > 0$, we have:

$$0 < g(\lambda_1) \leq g(\lambda_2) \leq \cdots \leq g(\lambda_n).$$

Finally, if $g(x)$ is nonincreasing, then the function $f_t(x) = t - g(x)$ is nondecreasing for all $t \in \mathbb{R}$. Fix $t > g(\lambda_n)$, so that

$$t - g(\lambda_1) \geq t - g(\lambda_2) \geq \cdots \geq t - g(\lambda_n) > 0,$$

that is,

$$f_t(\lambda_1) \geq f_t(\lambda_2) \geq \cdots \geq f_t(\lambda_n) > 0. \tag{2.15}$$

Now, if S is an extended Soules matrix, (2.15) and Theorem 2.10 imply that:

$$f_t(S\Lambda S^T) = tI - g(S\Lambda S^T) \geq 0.$$

Hence $g(S\Lambda S^T) = tI - f_t(S\Lambda S^T)$ is a nonsingular M-matrix. Conversely, if $g(S\Lambda S^T)$ is a nonsingular M-matrix, then for some $s > g(\lambda_n)$ and nonnegative matrix C we have $g(S\Lambda S^T) = sI - C$. But then:

$$C = sI - g(S\Lambda S^T) = S(sI - g(\Lambda))S^T = Sf_s(\Lambda)S^T,$$

hence appealing once more to Theorem 2.10 yields the result. □

An additional result appearing in [10, Corollary 2.4] that can be generalized in the same way as Corollary 2.11 is the following.

Corollary 2.12 *Let S be an orthogonal matrix and define $A = S\Lambda S^T$. Then for any $p \geq 0$, A^{-p} is a nonsingular M-matrix for every nonnegative diagonal matrix Λ with positive, non-increasing diagonal entries if and only if S is an extended Soules matrix. In particular, A^{-1} will always be an M-matrix.*

Proof. Choose $g(x) = 1/x^p$ in Corollary 2.11. □

Our final result is a special case of Theorem 2.10. We say a matrix A is *exponentially nonnegative* if

$$e^{tA} = \sum_{k=0}^{\infty} \frac{t^k A^k}{k!} \geq 0 \quad \text{for all } t \geq 0.$$

Corollary 2.13 *Let S be an orthogonal matrix. The following statements are equivalent.*

(i) S is an extended Soules matrix.

(ii) $S\Lambda S^T \geq 0$ for all nonnegative diagonal matrices Λ with non-increasing diagonal entries.

(iii) $S\Lambda S^T$ is exponentially nonnegative for all diagonal matrices Λ with non-increasing diagonal entries.

Proof. That $(i) \iff (ii)$ and $(i) \iff (iii)$ hold follows from taking $f(x) = x$ and $f(x) = e^x$, respectively, in Theorem 2.10. □

2.3.2 On Completely Positive Matrices

An $n \times n$ symmetric matrix A is *completely positive* if it can be represented as a product $A = BB^T$ where $B \geq 0$ is an $n \times m$ matrix. One basic, yet important (and unsolved) problem is to compute the smallest possible value of m (the number of columns of B) in the representation of $A = BB^T$. This smallest value of m is called the *cp-rank* of A. In [30], it is shown that if A can be diagonalized by a classical Soules matrix, i.e. *generated* by a classical Soules matrix, then *cp*-rank(A) = rank(A). In this section we prove that the same result is true if A is generated by an extended Soules matrix.

Let $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$ where $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. We say that Λ is a diagonal matrix with *non-increasing diagonal entries.* We begin with the following corollary of Theorem 2.6.

Corollary 2.14 *Let S be an $n \times n$ extended Soules matrix, and Λ a diagonal matrix with non-increasing diagonal entries. There are $n \times n$ permutation matrices P and Q, and an integer m, such that*

(i) PSQ is a direct sum of m classical Soules matrices $R_1, \ldots, R_m$, where R_i is $n_i \times n_i$, and

(ii) $Q^T \Lambda Q$ is a direct sum of m diagonal matrices $\Lambda_1, \ldots, \Lambda_m$, where Λ_i is $n_i \times n_i$, and each Λ_i has non-increasing diagonal entries.

Proof. If $S = [s_1, \ldots, s_n]$ is an extended Soules matrix, there exists a positive integer $m \leq n$ such that the columns $s_1 = s_{c_1}, s_{c_2}, \ldots, s_{c_m}$ are mono-signed. Let n_i be the cardinality of the set $\mathrm{supp}(s_{c_i})$, and define m-partitions $\{\mathscr{R}_1, \ldots, \mathscr{R}_m\}$ and $\{\mathscr{C}_1, \ldots, \mathscr{C}_m\}$ of n in accordance with Theorem 2.6 as follows: for each $i = 1, \ldots, m$,

$$\mathscr{R}_i = \{r_{i,1}, r_{i,2}, \ldots, r_{i,n_i}\} \quad \text{and} \quad \mathscr{C}_i = \{c_i = c_{i,1}, c_{i,2}, \ldots, c_{i,n_i}\}. \tag{2.16}$$

Let e_i denote the ith standard basis vector for $\mathbb{R}^n$, and define the permutation matrices P and Q as follows:

$$P = [e_{r_{1,1}}, e_{r_{1,2}}, \ldots, e_{r_{1,n_1}}, \ldots\ldots, e_{r_{m,1}}, e_{r_{m,2}}, \ldots, e_{r_{m,n_m}}]^T, \tag{2.17}$$

and

$$Q = [e_{c_{1,1}}, e_{c_{1,2}}, \ldots, e_{c_{1,n_1}}, \ldots\ldots, e_{c_{m,1}}, e_{c_{m,2}}, \ldots, e_{c_{m,n_m}}]. \tag{2.18}$$

Then, letting $m_j = \sum_{i=1}^{j} n_i$ and

$$\tilde{\mathscr{R}}_i = \tilde{\mathscr{C}}_i = \{m_{i-1}+1, \ldots, m_{i-1}+n_i\} = \{m_{i-1}+1, \ldots, m_i\},$$

observe that $(PSQ)[\tilde{\mathscr{R}}_i|\tilde{\mathscr{C}}_j] = S[\mathscr{R}_i|\mathscr{C}_j]$ for $i, j = 1, \ldots, m$. Hence, by Theorem 2.6, PSQ is a direct sum of m classical Soules matrices $R_1, \ldots, R_m$, where R_i is $n_i \times n_i$.

Additionally, if $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$ with $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, since $c_{i,1} < c_{i,2} < \cdots < c_{i,n_i}$, we have

$$\lambda_{c_{i,1}} \geq \lambda_{c_{i,2}} \geq \cdots \geq \lambda_{c_{i,n_i}}$$

for each $i = 1, \ldots, m$. Thus $Q^T \Lambda Q$ is a direct sum of diagonal matrices $\Lambda_1, \ldots, \Lambda_m$, where each $\Lambda_i = \mathrm{diag}(\lambda_{c_{i,1}}, \lambda_{c_{i,2}}, \ldots, \lambda_{c_{i,n_i}})$ has non-increasing diagonal entries. $\square$

Let S be an $n \times n$ extended Soules matrix, and Λ an $n \times n$ nonnegative diagonal matrix with non-increasing diagonal entries. We say the matrix $A = S\Lambda S^T$ is *generated by an extended Soules matrix.* The following result is proved in [30, Theorem 2.1].

Theorem 2.15 [30] *Let A be an $n \times n$ nonnegative matrix generated by a (classical) Soules matrix. Then cp$-$*$\mathrm{rank}(A) = \mathrm{rank}(A)$*.*

With Corollary 2.14 at hand, we are able to generalize Theorem 2.15 to matrices generated by extended Soules matrices.

Theorem 2.16 *Let $A \geq 0$ be an $n \times n$ matrix generated by an extended Soules matrix. Then cp$-$*$\mathrm{rank}(A) = \mathrm{rank}(A)$*.*

Proof. Let S be an $n \times n$ extended Soules matrix, $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_r, 0, \ldots, 0)$ with $\lambda_1 \geq \cdots \geq \lambda_r > 0$, and $A = S\Lambda S^T$. By Corollary 2.14, there are permutation matrices

P and Q such that PSQ is a direct sum of m Soules matrices $R_1, \dots, R_m$ where R_i is $n_i \times n_i$, and such that $Q^T \Lambda Q$ is the direct sum of m diagonal matrices $\Lambda_1, \dots, \Lambda_m$, each with non-increasing diagonal entries. Define $\tilde{A} = (PSQ)(Q^T \Lambda Q)(PSQ)^T$ and observe that $\tilde{A}$ is a direct sum of $R_i \Lambda_i R_i^T$, for $i = 1, \dots, m$. Let r_i denote the number of nonzero diagonal entries in Λ_i, and select the permutation matrix C such that the diagonal blocks $R_{j_1} \Lambda_{j_1} R_{j_1}^T, \dots, R_{j_m} \Lambda_{j_m} R_{j_m}^T$ of $C^T \tilde{A} C$ are ordered in non-increasing order according to r_i, i.e. $r_{j_1} \geq r_{j_2} \geq \cdots \geq r_{j_m}$. Let l be the largest index k such that $r_{j_k} > 0$. Then we have:

$$C^T \tilde{A} C = \begin{pmatrix} R_{j_1} \Lambda_{j_1} R_{j_1}^T & 0 & \cdots & \cdots & 0 \\ 0 & R_{j_2} \Lambda_{j_2} R_{j_2}^T & \cdots & \cdots & 0 \\ \vdots & \vdots & \ddots & & \vdots \\ 0 & 0 & \cdots & R_{j_l} \Lambda_{j_l} R_{j_l}^T & 0 \\ 0 & 0 & \cdots & 0 & 0 \end{pmatrix},$$

where the zero diagonal block is square with $n - (n_{j_1} + \cdots + n_{j_l}) = n_{j_{l+1}} + \cdots + n_{j_m}$ rows and columns. By Theorem 2.15, for each $k = 1, \dots, l$ there is a nonnegative $n_{j_k} \times r_{j_k}$ matrix B_{j_k} such that $R_{j_k} \Lambda_{j_k} R_{j_k}^T = B_{j_k} B_{j_k}^T$, hence we have $C^T \tilde{A} C = BB^T$, where:

$$B = \begin{pmatrix} B_{j_1} & 0 & \cdots & 0 \\ 0 & B_{j_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & B_{j_k} \\ 0 & 0 & \cdots & 0 \end{pmatrix}.$$

Since $\sum_{k=1}^{l} r_{j_k} = r$, it follows that B is $n \times r$. So, as $\tilde{A} = PAP^T$, it follows that $A = \tilde{B} \tilde{B}^T$ where $\tilde{B} = P^T C B \geq 0$ is $n \times r$, and thus the *cp*-rank and rank(A) are equal. This completes the proof. $\square$

2.4 Eigenvalues and Additional Classes of Orthogonal Matrices

We now turn to problem (2) mentioned in the opening paragraphs of this chapter. Namely, let $S = [s_1, \ldots, s_n] \in M_n$ be an orthogonal matrix and $\sigma = \{\lambda_1, \lambda_2, \ldots, \lambda_n\}$ be a sequence whose elements are ordered non-increasingly, $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \geq 0$, and suppose the pair (S, σ) satisfies (2.3):

$$\sum_{i=1}^{t} \lambda_i s_i s_i^T \geq 0 \quad t = 1, \ldots, n.$$

In the previous section, we considered σ to be fixed and described the structure of orthogonal matrices S satisfying (2.3) for $\lambda_1 = \lambda_2 = \cdots = \lambda_n = 1$ (or, as shown to be equivalent in Theorem 2.2, for every sequence σ such that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \geq 0$), and obtained a complete characterization of such matrices in Theorem 2.6.

Given an orthogonal matrix $S = [s_1, s_2, \ldots, s_n]$, we are interested here in describing the set of all points $(\lambda_1, \lambda_2, \ldots, \lambda_n) \in \mathbb{R}^n$ for which S satisfies (2.3) for each $t = 1, \ldots, n$. As a basis for preliminary results and further investigation into this problem, we make the following definitions and simplifying assumptions. Let

$$\Lambda_k = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_k, 0, \ldots, 0)$$

be $n \times n$ for $k = 1, \ldots, n$. Define:

$$\mathcal{S}_n = \{(\lambda_1, \lambda_2, \ldots, \lambda_n) \in \mathbb{R}^n : 1 = \lambda_1 \geq \cdots \geq \lambda_n \geq 0\}.$$

Associate with S the following two sequences $\mathcal{P}^n(S) = \{\mathcal{P}_1^n(S), \ldots, \mathcal{P}_n^n(S)\}$ and $\mathcal{Q}^n(S) = \{\mathcal{P}_1^n(S), \ldots, \mathcal{P}_n^n(S)\}$ of subsets of $\mathcal{S}_n$, where:

$$\mathcal{P}_k^n(S) = \left\{ (\lambda_1, \ldots, \lambda_k, 0, \ldots, 0) \in \mathcal{S}_n : S\Lambda_t S^T = \sum_{i=1}^{t} \lambda_i s_i s_i^T \geq 0, t = 1, \ldots, k \right\},$$

$$\mathcal{Q}_k^n(S) = \left\{ (\lambda_1, \ldots, \lambda_k, 0, \ldots, 0) \in \mathcal{S}_n : S\Lambda_k S^T = \sum_{i=1}^{k} \lambda_i s_i s_i^T \geq 0 \right\}.$$

Our primary goal in this section is thus to characterize $\mathcal{P}^n(S)$ which, since each $\mathcal{P}_k^n(S)$ is clearly convex, amounts to determining the vertices of $\mathcal{P}^n(S)$. Our introduction of the larger set $\mathcal{Q}^n(S)$, which is essentially the set of all solutions to the $n \times n$ symmetric NIEP for a given fixed basis, is just for comparison of results. For example, if

$$(\lambda_1, \lambda_2, \ldots, \lambda_{k-1}, \lambda_k, 0, \ldots, 0) \in \mathcal{P}_k^n(S),$$

then each of

$$(\lambda_1, 0, \ldots, 0), (\lambda_1, \lambda_2, \ldots, 0), \ldots, (\lambda_1, \lambda_2 \ldots, \lambda_{k-1}, 0, \ldots, 0) \in \mathcal{P}_k^n(S),$$

but the above statement is false in general if we replace $\mathcal{P}_k^n(S)$ with $\mathcal{Q}_k^n(S)$. In the same spirit as the above, we make the following observations regarding these sets.

Observation 2.17

(a) $\mathcal{P}_k^n(S) \neq \emptyset$, *i.e.* $(1, 0, \ldots, 0) \in \mathcal{P}_k^n(S)$ *for* $k = 1, \ldots, n$, *if and only if* s_1 *is mono-signed.*

(b) For any orthogonal $n \times n$ *matrix* S, $(1, 1, \ldots, 1) \in \mathcal{Q}_n^n(S)$.

(c) Fix $\lambda_1, \lambda_2, \ldots, \lambda_k$, *and define* $\mu_k = (\lambda_1, \lambda_2, \ldots, \lambda_k, 0, \ldots, 0) \in \mathcal{S}_n$. *If* $\mu_k \in \mathcal{Q}_k^n(S)$, *then* $\mu_k \in \mathcal{P}_k^n(S)$ *if and only if* $\mu_1, \ldots, \mu_{k-1} \in \mathcal{P}_k^n(S)$ *(i.e.* $\mu_j \in \mathcal{P}_j^n(S)$ *for* $j = 1, \ldots, k-1$*).*

(d) $\mathcal{P}_k^n(S) \subseteq \mathcal{P}_{k+1}^n(S)$ *for any orthogonal matrix* S*. In particular,* $\mathcal{P}_n^n(S) = \mathcal{P}^n(S)$.

(e) $\mathcal{P}_k^n(S) \subseteq \mathcal{Q}_k^n(S)$ *for each* $k = 1, \ldots, n$*. Equality holds for each* $k = 1, \ldots, n$ *if and only if* S *is an extended Soules matrix.*

Proof.

(a) If s_1 is mono-signed, then $s_1 s_1^T \geq 0$, hence $(1, 0, \ldots, 0) \in \mathcal{P}_k^n(S)$.

(b) That $(1, 1, \ldots, 1) \in \mathcal{Q}_n^n(S)$ is clear since $SIS^T = SS^T = I \geq 0$.

(c) The statement follows from the definitions of $\mathcal{P}_k^n(S)$ and $\mathcal{Q}_k^n(S)$. See also the comment preceding the statement of this observation.

(d) If $\mu = (\lambda_1, \ldots, \lambda_k, 0, \ldots, 0) \in \mathcal{P}_k^n(S)$, taking $\lambda_{k+1} = 0$ implies $\mu \in \mathcal{P}_{k+1}^n(S)$.

(e) The first part is obvious, and the second part follows from Theorem 2.2 and (b) above. $\square$

Since our main goal is to determine $\mathcal{P}^n(S)$, of immediate importance are the conditions under which we have equality or strict inclusion in Observation 2.17(d). To move toward an answer to this question, we note that $\mathcal{P}_k^n(S)$ contains points $(\lambda_1, \ldots, \lambda_k, 0, \ldots, 0)$ in $\mathcal{S}_n$ for which there are *at most* k positive coordinates. We call the maximal such k the *dimension* of $\mathcal{P}^n(S)$, and denote it by $\dim\mathcal{P}^n(S)$. Using the notation and definitions of this section, we obtain an immediate corollary of Theorem 2.1.

Theorem 2.18

(a) $\mathcal{P}_k^n(S) \neq \mathcal{P}_{k+1}^n(S)$ *if and only if* s_{k+1} *is mono-signed or has completely overlapping support with exactly one mono-signed column* s_j *for some* $1 \leq j < k+1$. *In particular, every multi-signed column* s_i *has completely overlapping support with exactly one mono-signed column* s_j *for* $j < i$, *or* s_1 *is strictly mono-signed, if and only if* $\dim\mathcal{P}^n(S) = n$.

(b) $\dim \mathcal{P}^n(S) = p$ *for some* $1 \leq p < n$*, i.e.* $\mathcal{P}^n_k(S) \subseteq \mathcal{P}^n_p(S)$ *for all* $k = 1, \ldots, n$*, if and only if* p *is the smallest index such that* s_{p+1} *is multi-signed and the support of* s_{p+1} *does not completely overlap that of* s_j *for any* $j = 1, \ldots, p$*.*

We illustrate Theorem 2.18 with an example.

Example 2.19 *Consider the following matrices.*

$$S_1 = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{7}} & -\frac{1}{\sqrt{42}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{7}} & \frac{1}{\sqrt{42}} \\ 0 & \frac{1}{\sqrt{3}} & \frac{2}{\sqrt{7}} & \frac{2}{\sqrt{42}} \\ 0 & 0 & \frac{1}{\sqrt{7}} & -\frac{6}{\sqrt{42}} \end{bmatrix}, \quad S_2 = \frac{1}{2}\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix}.$$

Both S_1 *and* S_2 *have mono-signed first columns, hence* $\mathcal{P}^4_1(S_1) = \mathcal{P}^4_1(S_1) = \{(1, 0, 0, 0)\}$*. Also, the support of the second column of* S_1 *does not completely overlap that of the first column, while in* S_2 *the first column is positive. Theorem 2.18 implies* $\dim \mathcal{P}^4(S_1) = 1$*,* $\mathcal{P}^4(S_1) = \mathcal{P}^4_1(S_1)$*, and* $\dim \mathcal{P}^4(S_2) = 4$*.* S_2 *is an example of a special orthogonal Hadamard matrix, which are discussed in further generality in 2.4.1.*

Note that if u and v are mono-signed and orthogonal vectors, they have supports that do not overlap, and hence there is a permutation matrix R such that the supports of Ru and Rv consist of consecutive integers, respectively. Hence Theorem 2.18(a) implies that if $\dim \mathcal{P}^n(S) = n$, there are permutation matrices R and T such that RST is a direct sum of blocks, with each block possessing a strictly mono-signed first column. We encountered this in the previous section in Theorem 2.6, in the case for which $(1, 1, \ldots, 1) \in \mathcal{P}^n_n(S)$.

We now consider the specification of $\mathcal{P}^n(S)$. Since each $S\Lambda_k S^T$ is symmetric and has nonnegative diagonal entries for $k = 1, \ldots, \dim \mathcal{P}^n(S)$, to determine $\mathcal{P}^n(S)$ is the same as specifying the feasible region determined by the following set of inequalities that are linear in λ_i:

$$\begin{cases} 1 = \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_k \geq 0 \\ (S\Lambda_t S^T)_{ij} = \sum_{r=1}^{t} \lambda_i s_{ir} s_{jr} \geq 0 \quad i,j = 1,\ldots,n, i < j; t = 1,\ldots,k \end{cases} \tag{2.19}$$

The number of inequalities in (2.19) is at most $\frac{kn(n-1)}{2} + k$; however, this number may be further reduced with knowledge of $\dim\mathcal{P}^n(S)$ and the sign pattern of S, in accordance with Theorem 2.18.

Remark 2.20 *In practice, we do not solve a separate system* (2.19) *for each k and take the union of the result to determine $\mathcal{P}^n(S)$. Rather, beginning with $k = 2$ (if s_1 is mono-signed), we collect for each successive k those inequalities which are independent of* (2.19) *for previous k. The resulting system then determines $\mathcal{P}^n(S)$. $\mathcal{P}_k^n(S)$ may then be constructed from the extreme points of $\mathcal{P}^n(S)$ for which the kth through the nth coordinates are zero.*

It turns out (see Theorem 2.21) that finding the extreme points of (2.19) is tantamount to determining $\mathcal{P}^n(S)$. To describe the potential forms the set $\mathcal{P}^n(S)$ may take, we require some additional notation and terminology, as set forth in [25, Chapters 2, 3]. Let V be a real finite-dimensional vector space, and S a subset of V. We say S is *convex* provided for all $x, y \in S$ we have $sx + (1-s)y \in S$ for all $0 \leq s \leq 1$. In particular, the convex set S contains all *convex linear combinations* of its elements, i.e. if $x_1, x_2, \ldots, x_m \in S$ then

$$z = s_1x_1 + s_2x_2 + \cdots + x_mx_m \in S$$

for any set of real numbers $s_1, s_2, \ldots, s_m$ such that

$$\sum_{i}^{m} s_i = 1.$$

Denote by $H\{x_1, x_2, \ldots, x_m\}$ the set of all convex linear combinations of $x_1, x_2, \ldots, x_m$. We call this set the *convex polyhedron with vertices* $x_1, x_2, \ldots, x_m$, or the *convex hull of* $x_1, x_2, \ldots, x_m$. A slightly more general notion emerges by considering the vector z above, where if we collect all vectors of the same form as z together with all multiples $w = \lambda z$ for $\lambda \geq 0$, the resulting set is called a *convex pyramid with vertices* $x_1, x_2, \ldots, x_m$, or the *positive hull of* $x_1, x_2, \ldots, x_m$.

To solve (2.19), we employ the general theory of linear inequalities developed in [25, Sec. 7.4], and summarize the main result proved there as follows. The resulting theorem is often called the "principle of boundary solutions."

Theorem 2.21 [25] *Let A be an $m \times n$ matrix of rank $r > 0$, x an $n \times 1$ column vector, and b an $m \times 1$ column vector. Consider the system of linear inequalities written in matrix form as follows:*

$$Ax - b \geq 0. \tag{2.20}$$

The set of solutions to (2.20) *is either empty or it is the sum $K = K_1 + K_2$ of a convex polyhedron K_1 and a convex pyramid K_2. Note that K_2 can be trivial here, since it consists of the solutions to the homogeneous system $Ax \geq 0$.*

Let $A^{(r)}$ be an $r \times r$ submatrix of A with rank r, and $x^{(r)}$ and $b^{(r)}$ both be $r \times 1$ subvectors of x and b indexed by the columns and rows of $A^{(r)}$, respectively. Then any solution of the system

$$A^{(r)}x^{(r)} - b^{(r)} = 0 \tag{2.21}$$

also satisfies (2.20)*. In particular, The convex polyhedron K_1 can be chosen so that its vertex vectors satisfy exactly one of the equations* (2.21)*.*

So, $\mathcal{P}^n(S)$ is thus the sum of a convex polyhedron and a convex pyramid, both of which can be determined by a finite number of vertices. The vertices are the extreme points of inequalities (2.19). In order to obtain the vertices of $\mathcal{P}^n(S)$, Theorem 2.21 suggests we take the following steps:

1. Use (2.19) to construct (2.20).

2. Compute $r = \operatorname{rank}(A)$.

3. Solve each $r \times r$ subsystem (2.21) obtained from (2.20) with rank r (if possible), and check that the solution satisfies (2.20).

We illustrate this process with an example as we conclude this section.

Example 2.22 *Consider the matrix S_2 in Example 2.19. For* $\Lambda = \operatorname{diag}(1, \lambda_2, \lambda_3, \lambda_4)$*, we have:*

$$S_2 \Lambda S_2^T = \frac{1}{4} \begin{bmatrix} 1+\lambda_2+\lambda_3+\lambda_4 & 1-\lambda_2+\lambda_3-\lambda_4 & 1+\lambda_2-\lambda_3-\lambda_4 & 1-\lambda_2-\lambda_3+\lambda_4 \\ 1-\lambda_2+\lambda_3-\lambda_4 & 1+\lambda_2+\lambda_3+\lambda_4 & 1-\lambda_2-\lambda_3+\lambda_4 & 1+\lambda_2-\lambda_3-\lambda_4 \\ 1+\lambda_2-\lambda_3-\lambda_4 & 1-\lambda_2-\lambda_3+\lambda_4 & 1+\lambda_2+\lambda_3+\lambda_4 & 1-\lambda_2+\lambda_3+\lambda_4 \\ 1-\lambda_2-\lambda_3+\lambda_4 & 1+\lambda_2-\lambda_3-\lambda_4 & 1-\lambda_2+\lambda_3-\lambda_4 & 1+\lambda_2+\lambda_3+\lambda_4 \end{bmatrix}$$

Proceeding according to Remark 2.20 once again, $\mathcal{P}^4(S_2)$ is determined by the system:

$$\begin{cases} 1 = \lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4 \geq 0, \\ 1 - \lambda_2 - \lambda_3 \geq 0 \end{cases} \tag{2.22}$$

Imposing (2.22) *and constructing* (2.20) *yields:*

$$Ax - b = \begin{bmatrix} -1 & 0 & 0 \\ 1 & -1 & 0 \\ 0 & 1 & -1 \\ 0 & 0 & 1 \\ -1 & -1 & 0 \end{bmatrix} \cdot \begin{bmatrix} \lambda_2 \\ \lambda_3 \\ \lambda_4 \end{bmatrix} - \begin{bmatrix} -1 \\ 0 \\ 0 \\ 0 \\ -1 \end{bmatrix} \geq 0. \tag{2.23}$$

Here $\mathrm{rank}(A) = 3$*, hence there are ten* 3×3 *subsystems of* (2.23) *to solve. Note that the subsystem of* (2.23) *determined by the row set* $\{1, 2, 5\}$ *has no solution, that of* $\{2, 3, 4\}$ *only the trivial solution, and the subsystems determined by* $\{1, 3, 4\}$, $\{1, 3, 5\}$, $\{1, 4, 5\}$, *and* $\{3, 4, 5\}$ *all have the same nontrivial solution. We summarize the result in the following table.*

Row Set(s)	$(\lambda_2, \lambda_3, \lambda_4)$
$\{2, 3, 4\}$	$(0, 0, 0)$
$\{1, 3, 4\}, \{1, 3, 5\}, \{1, 4, 5\}, \{3, 4, 5\}$	$(1, 0, 0)$
$\{2, 4, 5\}$	$(1/2, 1/2, 0)$
$\{2, 3, 5\}$	$(1/2, 1/2, 1/2)$
$\{1, 2, 4\}$	$(1, 1, 0)$
$\{1, 2, 3\}$	$(1, 1, 1)$

Only the first four solutions above satisfy (2.23)*, hence by Theorem 2.21:*

$$\mathcal{P}^4(S_2) = H\{(1, 0, 0, 0), (1, 1, 0, 0), (1, 1/2, 1/2, 0), (1, 1/2, 1/2, 1/2)\}.$$

2.4.1 On Special Orthogonal Hadamard Matrices

A square matrix H whose entries consist of $+1$ or -1 is said to be a *Hadamard matrix of order* n if $HH^T = nI$, i.e. if distinct columns of H are orthogonal and if the Euclidean norm of each column is equal to n. Any matrix satisfying these properties cannot have odd order, and so n must be even. An interesting open problem for these matrices (which we do not address here) called the Hadamard Conjecture is that for every k there is a Hadamard matrix of order $4k$.

For every Hadamard matrix H, notice that the matrix $S = \frac{1}{\sqrt{n}}H$ is an orthogonal matrix, what we shall call an *orthogonal Hadamard matrix*. For example, the following two matrices are orthogonal Hadamard matrices:

$$S_1 = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \qquad S_2 = \frac{1}{2}\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix}.$$

Recall that the matrix S_2 was considered in Section 2.4 in Examples 2.19 and 2.22.

Using a construction originally devised by Sylvester, if H is any $n \times n$ Hadamard matrix, we may construct a $2n \times 2n$ Hadamard matrix as follows:

$$\begin{bmatrix} S & S \\ S & -S \end{bmatrix}.$$

Observe that if we take S to be the above 2×2 matrix S_1, using this construction technique gives rise to the 4×4 matrix S_2 above. Defining the $2^{m+1} \times 2^{m+1}$ matrix

$$S_{m+1} = \frac{1}{\sqrt{2}}\begin{bmatrix} S_m & S_m \\ S_m & -S_m \end{bmatrix}, \quad m = 1, 2, \ldots$$

with S_1 and S_2 given above, we obtain an infinite sequence of orthogonal Hadamard matrices, which we shall call *special orthogonal Hadamard matrices*. The purpose of this section is to determine the inequalities yielding $\mathcal{P}^{2^m}(S_m)$ for an arbitrary integer $m \geq 1$.

It is interesting to note that S_m, and hence $A_j = S_m \Lambda_m S_m^T$, is symmetric for each $m \geq 1$. Another interesting fact is that A_m, in addition to being symmetric, is also *anti-symmetric*, that is, symmetric about its anti-diagonal. Although these two facts, symmetry and anti-symmetry, are useful to note, a more important fact for the problem at hand is that each row of A_m contains precisely the same entries as the first row. It is this stronger result which we now prove.

Theorem 2.23 *Consider the sequence S_m for $m \geq 1$ as defined above, and let $\Lambda_m = \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_{2^m})$ be any $2^m \times 2^m$ diagonal matrix. Then the matrix $A_m = [a_{i,j}^m] = S_m \Lambda_m S_m^T$ is completely determined by its first row; that is, there is an l such that $a_{i,j}^m = a_{1,l}^m$ for every i, j with $1 < i \leq 2^m$.*

Proof. We proceed by induction on m. Observe that:

$$A_1 = \frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}\begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} \lambda_1 + \lambda_2 & \lambda_1 - \lambda_2 \\ \lambda_1 - \lambda_2 & \lambda_1 + \lambda_2 \end{bmatrix}.$$

Now assume $A_m = S_m \Lambda_m S_m^T$ is completely determined by its first row, and consider A_{m+1}. Partition Λ_{m+1} as follows:

$$\Lambda_{m+1} = \begin{bmatrix} \Lambda_1^{m+1} & 0 \\ 0 & \Lambda_2^{m+1} \end{bmatrix},$$

where Λ_1^{m+1} and Λ_2^{m+1} are $2^m \times 2^m$ diagonal matrices. Using our definition of S_{m+1}, we compute:

$$\begin{aligned} A_{m+1} &= \begin{bmatrix} S_m & S_m \\ S_m & -S_m \end{bmatrix} \begin{bmatrix} \Lambda_1^{m+1} & 0 \\ 0 & \Lambda_2^{m+1} \end{bmatrix} \begin{bmatrix} S_m & S_m \\ S_m & -S_m \end{bmatrix} \\ &= \begin{bmatrix} S_m(\Lambda_1^{m+1} + \Lambda_2^{m+1})S_m^T & S_m(\Lambda_1^{m+1} - \Lambda_2^{m+1})S_m^T \\ S_m(\Lambda_1^{m+1} - \Lambda_2^{m+1})S_m^T & S_m(\Lambda_1^{m+1} + \Lambda_2^{m+1})S_m^T \end{bmatrix}. \end{aligned} \tag{2.24}$$

By our induction hypothesis, $S_m(\Lambda_1^{m+1} + \Lambda_2^{m+1})S_k^T$ and $S_m(\Lambda_1^{m+1} - \Lambda_2^{m+1})S_m^T$ are completely determined by their first rows, and since concatenating these rows make up the first row of A_{m+1}, the same is true of A_{m+1}. This completes the proof. $\square$

The clear advantage of Theorem 2.23 in achieving our aforementioned goal is that we need only consider the first row of $S_m\Lambda_t S_m^T$ in determining $\mathcal{P}^{2^m}(S_m)$. Moreover, as our next result shows, if we know $\mathcal{P}^{2^{m-1}}(S_{m-1})$, we need only append 2^m zeros to each of its points to obtain $\mathcal{P}_k^{2^m}(S_m)$ for $k = 1, \ldots, 2^m$, and thus limit our attention to the first rows of $S_m\Lambda_t S_m^T$ for $t > 2^{m-1}$.

Theorem 2.24 *Define $\hat{\mathcal{P}}_k^{2^m}(S_m)$ as a subset of $\mathbb{R}^{2^{m+1}}$ by appending 2^m zeros to each point of $\mathcal{P}_k^{2^m}(S_m)$, for $m \geq 1$, $k = 1, \ldots, 2^m$. Then for each $k = 1, \ldots, 2^{m+1}$, we have $\hat{\mathcal{P}}_k^{2^m}(S_m) \subseteq \mathcal{P}_k^{2^{m+1}}(S_{m+1})$, with equality if and only if $1 \leq k \leq 2^m$.*

Proof. For $k = 1, \ldots, 2^m$, let $\Lambda_k = \mathrm{diag}(1, \lambda_2, \ldots, \lambda_k, 0, \ldots, 0)$ be $2^m \times 2^m$, and define the $2^{m+1} \times 2^{m+1}$ matrix:

$$\hat{\Lambda}_k = \begin{bmatrix} \Lambda_k & 0 \\ 0 & 0 \end{bmatrix}.$$

Using our definition of S_m as in (2.24), as well as Theorem 2.23, it follows that:

$$(S_{m+1}\Lambda_k S_{m+1}^T)_{1,*} = [(S_m\Lambda_k S_m^T)_{1,*}, (S_m\Lambda_k S_m^T)_{1,*}],$$

which is nonnegative if and only if $(S_m\Lambda_k S_m^T)_{1,*} \geq 0$. Since $(S_m\Lambda_k S_m^T)_{1,*} \geq 0$, we have $\hat{\mathcal{P}}_k^{2^m}(S_m) = \mathcal{P}_k^{2^{m+1}}(S_{m+1})$ for each $k = 1, \dots, 2^m$. That $\hat{\mathcal{P}}_k^{2^m}(S_m) \subseteq \mathcal{P}_k^{2^{m+1}}(S_{m+1})$ for $k = 2^m, 2^m+1, \dots, 2^{m+1}$ follows from Observation 2.17(d) and Theorem 2.18(a). $\square$

While Theorems 2.23 and 2.24 are useful in limiting the number of inequalities we must consider in (2.19), and since there are potentially 2^m distinct first-row entries of $S_m\Lambda_t S_m^T$, to proceed requires a deeper consideration of the sign pattern of S_m. To this end, observe that an additional consequence of Theorems 2.23 and 2.24 (together with symmetry) is:

$$(S_m\Lambda_k S_m^T)_{1,*}^T \geq 0 \quad \text{if and only if} \quad 2^{m/2} S_m x_k \geq 0,$$

where $x_k = [1, \lambda_2, \lambda_3, \dots, \lambda_k, 0, \dots, 0]^T$. So, as $1 \geq \lambda_2 \geq \cdots \geq \lambda_k \geq 0$, of particular concern are those rows of S_m for which there are more λ_i's being subtracted in computing $S_m x_k$ than being added, and this is determined completely by the sign pattern of the first k columns of S_m.

Although we cannot explicitly specify the jth row of S_m (or even its sign pattern) in general, we can, however, say something about the distribution of positive and negative entries in S_m, particularly its first columns. This is the content of our next two results.

Theorem 2.25 *Consider the sequences S_m and $m \geq 1$. For each $j = 0, \dots, m-1$, the row(s) of S_m indexed by $(2l-1)\cdot 2^j + 1$ for $l = 1, \dots, 2^{m-j-1}$, have exactly 2^j positive entries in the first 2^j columns. Also, the first 2^{m-1} entries of row $2^{m-1}+1$ are positive, while the rest are negative, and the first row of S_m contains 2^m positive entries.*

Proof. We proceed by induction on m. If $m = 1$ the assertion is trivial. Suppose the assertion holds for S_m and consider S_{m+1}. By definition of S_m, it follows that for $j = 0, \ldots, m-1$ the rows of S_{m+1} indexed by $(2l-1) \cdot 2^j + 1$ for $l = 1, \ldots, 2^{m-j-1}, 2^{m-j-1}+1, \ldots, 2 \cdot 2^{m-j-1}$, i.e. for $l = 1, \ldots, 2^{m-j}$, have exactly 2^j positive entries in the first 2^j columns. Since the first row of S_m contains 2^m positive entries, the first 2^m entries of row $2^m + 1$ of S_{m+1} are positive, while the rest are negative. Finally, the first row of S_{m+1} contains 2^{m+1} entries. This completes the proof. $\square$

Theorem 2.26 *Consider row s, $1 < s \neq 2^{m-1}$, of S_m for $m \geq 2$, and let row s have exactly 2^j positive entries in its first 2^j columns. Then the entry in the last column belongs to a block of 2^j consecutive entries of the same sign. Moreover, every entry of this row belongs to a block of entries of the same sign containing 2^j or 2^{j+1} entries.*

Proof. Note the assertion holds for the rows s of S_m that are excluded: rows 1 and 2^{m-1}. We proceed by induction on m. For $m = 2$ the assertion holds by observing S_2. Suppose the assertion is true for S_m and consider S_{m+1}. That is, By definition of S_m, the result holds for the first 2^m columns of S_{m+1}, hence the final entry of S_m belongs to a block of 2^j consecutive entries. The row s satisfies either $1 \neq s < 2^m$ or $s > 2^m$. In the former case, the entry in column 2^m belongs to a group of 2^j consecutive entries if it is negative, or a group of 2^{j+1} consecutive entries if it is positive. In the latter case, we interchange "positive" and "negative" in the previous argument. All other entries satisfy the induction hypothesis, and so our proof is complete. $\square$

We say that two rows of S_m are *equivalent* provided they have the same number 2^j of positive entries in its first 2^j columns, for $0 \leq j \leq m$. This defines an equivalence relation on the rows of S_m. We select representatives of these $m+1$ equivalence classes as follows:

$$
\begin{array}{rc}
j = 0: & [+,-,-,+,*,\dots,*] \\
j = 1: & [+,+,-,-,-,-,+,*,\dots,*] \\
\vdots & \vdots \\
j = t: & [\underbrace{+,\dots,+}_{2^t \text{ terms}},\underbrace{-,\dots,-}_{2^{t+1} \text{ terms}},+,*,\dots,*] \\
\vdots & \vdots \\
j = m-2: & [\underbrace{+,\dots,+}_{2^{m-2} \text{ terms}},\underbrace{-,\dots,-}_{2^{m-1} \text{ terms}},\underbrace{+,\dots,+}_{2^{m-2} \text{ terms}}] \\
j = m-1: & [\underbrace{+,\dots,+}_{2^{m-1} \text{ terms}},\underbrace{-,\dots,-}_{2^{m-1} \text{ terms}}] \\
j = m: & [+,\dots,+]
\end{array}
$$

Note that for $j = m-1$ and $j = m$, the rows shown above are the only elements of the respective classes, and all other equivalence classes have 2^{m-j-1} members (by Theorem 2.25).

To further analyze the sign pattern of S_m, and hence each equivalence class of its rows, we introduce the following sequence of matrices N_m, for $m \geq 1$. Each N_m is $2^m \times 2^m$, which via multiplication will yield successive row sums of $2^{m/2}S_m$:

$$
N_1 = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}, \quad N_{m+1} = \begin{bmatrix} N_m & O_m \\ 0 & N_m \end{bmatrix}, \quad m = 1, 2, \dots
$$

where O_m is a $2^m \times 2^m$ matrix of 1's. The kth column of the matrix $R_m = 2^{m/2}S_mN_m$ is thus the sum of the first k columns of $2^{m/2}S_m$, for $k = 1, \dots, 2^m$. Inequalities we must impose on $2^{m/2}S_mx_k$ in addition to $1 \geq \lambda_2 \geq \cdots \geq \lambda_k \geq 0$ then result from encountering negative entries in or prior to the kth column in a given row of R_m. If a row of R_m has a negative entry, we call the corresponding row of S_m *sign-imbalanced*, since it indicates that at the column for which the negative entry appears in the row, there are more negative entries than positive entries. A row of R_m that is nonnegative is thus called *sign-balanced*. Interestingly, we can explicitly identify the smallest entry in each sign-imbalanced row.

Theorem 2.27 *Consider the sequence $R_m = 2^{m/2} S_m N_m$ for $m \geq 2$ (note that $R_1 \geq 0$). For each $j = 0, \ldots, m-2$, the row(s) indexed by $(3+2l)2^j + 1$ for $l = 0, \ldots, 2^{m-j-1} - 2$, are sign-imbalanced, and contain both -2^j and 2^j, which are the smallest and largest entries in this row. All other rows of R_m are sign-balanced; moreover, row $2^{m-1} + 1$ is nonnegative and has largest entry 2^{m-1}.*

Proof. We proceed by induction on m. Observe that:

$$R_1 = \begin{bmatrix} 1 & 2 \\ 1 & 0 \end{bmatrix} \geq 0,$$

and

$$R_2 = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 1 & 0 & 1 & 0 \\ 1 & 2 & 1 & 0 \\ 1 & 0 & -1 & 0 \end{bmatrix}.$$

Notice that both $1 = 2^0$ and $-1 = -2^0$ appear in row $4 = (3 + 2 \cdot 0)2^0 + 1$, all other rows of R_2 are nonnegative, and the largest entry of row $3 = 2^{2-0-1} + 1$ is $2 = 2^{2-0-1}$.

Suppose the assertion holds for R_m and consider R_{m+1}. A computation reveals:

$$R_{m+1} = \begin{bmatrix} R_m & 2^{m/2} S_m O_m + R_m \\ R_m & 2^{m/2} S_m O_m - R_m \end{bmatrix}.$$

Notice:

$$2^{m/2} S_m O_m = \begin{bmatrix} 2^m & \cdots & 2^m \\ 0 & \cdots & 0 \\ \vdots & & \vdots \\ 0 & \cdots & 0 \end{bmatrix},$$

and so partitioning R_m as follows:

$$R_m = \left[\begin{array}{ccc} 1 & \cdots & 2^m \\ \hline & \hat{R}_m & \end{array}\right]$$

where $\hat{R}_m$ is $(2^m - 1) \times 2^m$, we have:

$$R_{m+1} = \left[\begin{array}{ccc|ccc} 1 & \cdots & 2^m & 2^m+1 & \cdots & 2^{m+1} \\ \hline & \hat{R}_m & & & \hat{R}_m & \\ \hline 1 & \cdots & 2^m & 2^m-1 & \cdots & 0 \\ \hline & \hat{R}_m & & & -\hat{R}_m & \end{array}\right]. \tag{2.25}$$

So we need only consider the last $2^m - 1$ rows of R_{m+1}. Specifically, from the above computation it is clear that for each $j = 0, \ldots, m-2$, the row of R_{m+1} indexed by $(3+2l)2^j + 1$ for $l = 0, \ldots, 2^{m-j-1} - 2$, contain both -2^j and 2^j, and row 2^{m-1} of $\hat{R}_m$ is nonnegative and contains the entry 2^{m-1}. Thus, row $2^m + 2^{m-1} + 1 = (3+2l)2^j + 1$ for $l = 0$ and $j = m-1$ of R_{m+1} contains both 2^{m-1} and -2^{m-1}. Finally, notice that row 2^m+1 of R_{m+1} is nonnegative and contains the entry 2^m. This completes the proof.□

Note that, by Theorem 2.26, a row of S_m with 2^j positive entries in the first 2^j columns contains positive and negative entries in blocks of 2^j or 2^{j+1}. We now prove that a row of R_m containing smallest entry -2^j has the same index as a row of S_m containing a block of 2^j positive entries in its first 2^j columns.

Theorem 2.28 *Consider the sequences S_m and $m \geq 2$. For each $j = 0, \ldots, m-2$, the row(s) of S_m indexed by $(3+2l)2^j + 1$ for $l = 0, \ldots, 2^{m-j-1} - 2$, have exactly 2^j positive entries in the first 2^j columns. In particular, the first 2^{m-1} entries of row $2^{m-1}+1$ are positive, and the rest are negative.*

Proof. We proceed by induction on m. For S_2, row $4 = (3 + 2 \cdot 0)2^0 + 1$ has $1 = 2^0$ positive entries in its first 2^0 column. Suppose the assertion holds for S_m and consider S_{m+1}. By definition of S_{m+1} and by our assumption on S_m, and since $j \leq m-2$, rows $(3+2l)2^j + 1$, for $l = 0, \ldots, 2^{m-j-1} - 2 + 2^{m-j-1}$, i.e. $l = 0, \ldots, 2^{m-j} - 2$, have exactly 2^j positive entries in the first 2^j columns, and the proof is complete. $\square$

Before proceeding to our main result, we make a few comments. Consider the equivalence class of rows of S_m containing exactly 2^j positive entries in its first 2^j columns. Applying Theorem 2.26 to this equivalence class gives two possibilities:

$$[\underbrace{+,\ldots,+}_{2^j \text{ terms}},\underbrace{-,\ldots,-}_{2^j \text{ terms}},\underbrace{-,\ldots,-}_{2^j \text{ terms}},*,\ldots,*], \qquad [\underbrace{+,\ldots,+}_{2^j \text{ terms}},\underbrace{-,\ldots,-}_{2^j \text{ terms}},\underbrace{+,\ldots,+}_{2^j \text{ terms}},*,\ldots,*].$$

The first of these is clearly sign-imbalanced. Considering $\mathcal{P}_{3\cdot 2^j}^{2^m}(S_m)$, we must therefore require:

$$1 + \lambda_2 + \cdots + \lambda_{2^j} - \lambda_{2^j+1} - \cdots - \lambda_{3\cdot 2^j} = \sum_{i=1}^{2^j} \lambda_i - \sum_{i=2^j+1}^{3\cdot 2^j} \lambda_i \geq 0.$$

By Theorems 2.27 and 2.28, each sign-imbalanced row of S_m in this equivalence class corresponds to a row of R_m for which the smallest entry is -2^j. Thus, upon consideration of the corresponding entries of $2^{m/2} S_m x_k$ for $m \geq j+2$ and $k \geq 3 \cdot 2^j$, we may[1] equate the above inequality holding with adding 2^j to each row with smallest term -2^j in

[1] That this statement is true may be verified by hand; a rigorous proof remains to be found.

R_m, which results in this row becoming sign-balanced. So, the above inequality implies $2^{m/2} S_m x_k \geq 0$ for all $3 \cdot 2^j \leq k \leq 2^m$ and each $m \geq j+2$. Moreover, if the second sign pattern above is sign-imbalanced, it's corresponding row of R_m has smallest entry -2^j; however, observe that if we use the above inequality, the corresponding entry of $2^{m/2} S_m x_k$ for $m \geq j+2$ and $k = 3 \cdot 2^j$ is:

$$\sum_{i=1}^{2^j} \lambda_i - \sum_{i=2^j+1}^{2^{j+1}} \lambda_i + \sum_{i=2^{j+1}+1}^{3 \cdot 2^j} \lambda_i.$$

If we add and subtract the third term above, the following inequality is clear:

$$\sum_{i=1}^{2^j} \lambda_i - \sum_{i=2^j+1}^{3 \cdot 2^j} \lambda_i + 2 \cdot \sum_{i=2^{j+1}+1}^{3 \cdot 2^j} \lambda_i \geq 0.$$

Again, notice that adding and subtracting the third term and combining as above is equivalent to adding 2^j to each term of the corresponding row of R_m, so that the row becomes sign-balanced, hence $2^{m/2} S_m x_k \geq 0$ for all $3 \cdot 2^j \leq k \leq 2^m$ and each $m \geq j+2$. Collecting the above inequalities for $j = 0, \ldots, m-2$, i.e. one for each equivalence class, establishes our main theorem.

Theorem 2.29 *Consider the sequence S_m, $m \geq 1$, as defined above. Then* (2.19) *for $\mathcal{P}_k^{2^m}(S_m)$ for $k = 1, 2, \ldots, 2^m$ becomes:*

$$\begin{cases} 1 = \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_k \geq 0, \\ \sum_{i=1}^{2^s} \lambda_i - \sum_{i=2^s+1}^{3 \cdot 2^s} \lambda_i \geq 0, \qquad s = 0, 1, \ldots, m-2, \end{cases} \tag{2.26}$$

where, for indices s such that $2^s > k$, we have $\lambda_t = 0$.

We now consider the solution $\mathcal{P}^{2^m}(S_m)$ of system (2.26). Notice that if we write

(2.26) in matrix form, we have:

$$Ax - b = \begin{bmatrix} -1 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 \\ 1 & -1 & 0 & 0 & \cdots & \cdots & 0 & 0 \\ 0 & 1 & -1 & 0 & \cdots & \cdots & 0 & 0 \\ 0 & 0 & 1 & -1 & \cdots & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \ddots & \cdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \cdots & 1 & -1 \\ 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 1 \\ -1 & -1 & 0 & 0 & \cdots & \cdots & 0 & 0 \\ 1 & -1 & -1 & -1 & -1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & 1 & 1 & \cdots & \cdots & -1 & -1 \end{bmatrix} \begin{bmatrix} \lambda_2 \\ \lambda_3 \\ \lambda_4 \\ \lambda_5 \\ \vdots \\ \lambda_{2^m-1} \\ \lambda_{2^m} \end{bmatrix} - \begin{bmatrix} -1 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ -1 \\ -1 \\ \vdots \\ -1 \end{bmatrix} \geq 0.$$

The matrix A is $(2^m + m - 1) \times (2^m - 1)$, and $\text{rank}(A) = 2^m - 1$, so by Theorem 2.21, the solution set $\mathcal{P}^{2^m}(S_m)$ consists of a convex polyhedron. Recall that for $m = 2$, $\mathcal{P}^4(S_2)$ was obtained in Example 2.22. Although determining (2.26), and not its general solution (the extreme points of $\mathcal{P}^{2^m}(S_m)$ for general m) was the purpose of this section, it is the goal of future research to obtain a general form of the solution to (2.26), if one exists, or to prove that no useful closed-form exists.

To solve (2.26) for $m = 3$, we implement the MATLAB function `sohad` (see Appendix A.1), which was written for this purpose. This MATLAB function takes as input the value of m, and follows precisely the steps outlined after Theorem 2.21 using (2.26). The function's output is the set of extreme points of $\mathcal{P}^{2^m}_{3\cdot 2^{m-2}}(S_m)$ written as a matrix with each extreme point a column. The program runs in time exponential according to m, and is impractical for $m \geq 7$. For $m = 3$, we see that $\mathcal{P}^8(S_3)$ is the convex hull of 17 points:

$$
\begin{aligned}
\mathcal{P}^8(S_3) = H\{&(1,0,0,0,0,0,0,0),(1,1,0,0,0,0,0,0),(1,1/2,1/2,0,0,0,0,0),\\
&(1,1/2,1/2,1/2,0,0,0,0),(1,1/2,1/2,1/2,1/2,0,0,0),\\
&(1,1/3,1/3,1/3,1/3,0,0,0),(1,1/2,1/2,1/3,1/3,1/3,0,0,0),\\
&(1,1/2,1/2,1/2,1/4,1/4,0,0,0),(1,3/5,2/5,2/5,2/5,2/5,0,0,0)\\
&(1,1/3,1/3,1/3,1/3,1/3,1/3,0),(1,1/2,1/2,1/3,1/3,1/3,1/3,0)\\
&(1,1/2,1/2,1/2,1/4,1/4,1/4,0),(1,3/5,2/5,2/5,2/5,2/5,2/5,0),\\
&(1,1/3,1/3,1/3,1/3,1/3,1/3,1/3),(1,1/2,1/2,1/3,1/3,1/3,1/3,1/3)\\
&(1,1/2,1/2,1/2,1/4,1/4,1/4,1/4),(1,3/5,2/5,2/5,2/5,2/5,2/5,2/5)\}
\end{aligned}
$$

For $m = 4$, $\mathcal{P}^{16}(S_4)$ is the convex hull of 184 points, which we do not present here.

2.5 Conclusion

In this chapter we were able to obtain an important characterization of nonnegative symmetric matrices for which each successive partial sum of the spectral decomposition is a nonnegative matrix. Specifically, we have shown that the widely known class of orthogonal matrices known as Soules matrices, which satisfy this property in a very specific way, are actually a subclass of a larger set of orthogonal matrices, which we call extended Soules matrices. Soules matrices are thus referred to as classical Soules matrices, and we prove that each extended Soules matrix is a limit of a sequence of classical Soules matrices. Upon obtaining a characterization of extended Soules matrices, we examined nonnegativity of matrix functions whose inputs are matrices generated by extended Soules matrices. As an additional application, we proved that every matrix generated by an extended Soules matrix is completely positive, with rank equal to the *cp*-rank.

Given a symmetric matrix which satisfies the nonnegative successive partial sum property, the over-arching theme of this chapter was to examine two basic problems: fix the coefficients and vary the orthogonal matrix, or vary the coefficients and fix the orthogonal matrix. Our best general result linking both problems is given by the Main Theorem - its main drawback is that it does not specify any relationship among the coefficients that is certain to prevail in specific examples. A major step toward a general solution to the first problem is that of extended Soules matrices, which the first half of the chapter was devoted to. As a first step toward that of the second problem, which amounts in scope to the same type of problem as the SNIEP and requires the solution of a system of linear inequalities, we obtain a characterization for the coefficients of a special class of orthogonal Hadamard matrices. A closed-form solution set for the coefficients of such matrices seems imminent, but requires further research. An investigation of this set of coefficients for other classes of orthogonal matrices may also engender further interesting results in future research as well.

Chapter 3

The Nonnegative Inverse Eigenvalue Problem for Normal Matrices

Given a list $\sigma = \{\lambda_1, \lambda_2, \ldots, \lambda_n\}$ of n complex numbers, the *Nonnegative Inverse Eigenvalue Problem* (NIEP) seeks necessary and sufficient conditions for the existence of a nonnegative $n \times n$ matrix A such that σ is the spectrum of A. This problem is completely solved only for $n = 3$ and $n = 4$, and only partially for $n = 5$. While the NIEP remains open in general, several necessary and a profusion of sufficient conditions are known, some of which we discuss in this chapter.

We do not attempt here an adequate summary of known results related to the NIEP, nor do we wish to exemplify the varied and numerous applications, subproblems, extensions, or methods of numerical solution. For a recent thorough, yet brief, summary of results related to the NIEP, which also includes an extensive bibliography of papers dealing with the NIEP as stated above, see [9]; for a complete and comprehensive consideration of the NIEP, including an analysis of each of its many subproblems, applications, and numerical solutions, see [7]. The topic of this chapter is a special case of the NIEP, the *Normal NIEP* (NNIEP), which seeks necessary and sufficient conditions for the existence of a normal nonnegative matrix with spectrum σ.

We begin in Section 3.1 with a brief overview of the NIEP, specifically we outline necessary conditions, and some sufficient conditions for general NIEP. In turn, this will lead us in Section 3.2 to a discussion of known sufficient conditions for the NNIEP, the compendium of which to our knowledge has not been collected in a single source before. Now, if N is a normal matrix and $N = S + K$ with symmetric S and skew-symmetric K, that the condition $N \geq 0$ places certain restrictions on the possible sign-patterns of K is proved in Section 3.3. An analysis of these sign patterns, specifically the potential eigenvectors associated with the given spectrum, is then undertaken to solve the NNIEP for $n = 3$, and to provide a partial solution to the NNIEP for $n = 4$. The chapter is concluded with a discussion of questions raised in the current work, and directions for further research into the NNIEP.

3.1 Overview of the NIEP

3.1.1 Necessary Conditions

We begin with the following, now somewhat classical, conditions on σ which are necessary for the existence of a nonnegative matrix A with spectrum σ.

Theorem 3.1 *Let $A \geq 0$ be $n \times n$ with $\sigma(A) = \{\lambda_1, \lambda_2, \ldots, \lambda_n\}$. Then:*

(a) $\rho(A) = \max\{|\lambda_i| : \lambda_i \in \sigma(A)\} \in \sigma(A)$.

(b) $\sigma(A) = \overline{\sigma(A)}$.

(c) $s_k = \sum_{i=1}^{n} \lambda_i^k \geq 0,\ k = 1, 2, \ldots$.

(d) $s_k^m \leq n^{m-1} s_{km},\ k, m = 1, 2, \ldots$.

Proof.

(a) The statement follows from the Perron-Frobenius Theorem.

(b) The characteristic polynomial of A has real coefficients, hence any complex eigenvalues must occur in conjugate pairs.

(c) Since $s_k = \mathrm{tr}(A^k)$, the result follows from $A^k \geq 0$, $k = 1, 2, \ldots$.

(d) Let $A = D + C$ where $D = \mathrm{diag}(a_{11}, a_{22}, \ldots, a_{nn})$. Since $A \geq 0$:

$$A^m = (D + C)^m \geq D^m + C^m \geq 0.$$

It follows that:

$$s_m = \mathrm{tr}(A^m) \geq \mathrm{tr}(D^m) + \mathrm{tr}(C^m) = \sum_{i=1}^{n} a_{ii}^m + \mathrm{tr}(C^m). \tag{3.1}$$

Recall Hölder's Inequality: for any positive p, q satisfying $\frac{1}{p} + \frac{1}{q} = 1$:

$$\sum_{i=1}^{n} |x_i y_i| \leq \left(\sum_{i=1}^{n} |x_i|^p \right)^{1/p} \cdot \left(\sum_{i=1}^{n} |y_i|^q \right)^{1/q}.$$

Taking $p = \frac{m}{m-1}$, $q = m$, $x_i = 1$, and $y_i = a_{ii}$, we have:

$$s_1 = \sum_{i=1}^{n} a_{ii} = \sum_{i=1}^{n} 1 \cdot a_{ii} \leq \left(\sum_{i=1}^{n} 1 \right)^{\frac{m-1}{m}} \cdot \left(\sum_{i=1}^{n} a_{ii}^m \right)^{\frac{1}{m}} = n^{\frac{m-1}{m}} \left(\sum_{i=1}^{n} a_{ii}^m \right)^{\frac{1}{m}}.$$

Hence multiplying (3.1) by n^{m-1} and applying the inequality obtained from the above by raising both sides to the power m yields:

$$n^{m-1} s_m \geq n^{m-1} \sum_{i=1}^{n} a_{ii}^m + n^{m-1} \mathrm{tr}(C^{km}) \geq s_1^m + n^{m-1} \mathrm{tr}(C^{km}).$$

Thus $s_1^m \leq n^{m-1} s_m$, and we have proved the inequality in the case $k = 1$. Applying the above to the matrix $B = A^k$ yields the remaining cases. $\square$

We remark that in [12, Theorem 1] Friedland proved that any set σ of complex numbers satisfying Theorem 3.1(c) must also satisfy 3.1(a). Also, conditions 3.1(d) are called the "JLL Conditions," so-named since they were proved independently by Loewy and London [18], and Johnson [15]. We also observe that further necessary conditions on the coefficients of the characteristic polynomial of A (hence, the s_k's) were recently obtained in [36, Theorem 3] using graph theoretic techniques.

Remark 3.2 *The conditions in Theorem 3.1 are sufficient for the existence of a nonnegative matrix A with spectrum σ for $n = 3$, as is shown in Theorem 3.25 below. This is false for $n \geq 4$. To see this, suppose $\sigma(A) = \{\sqrt{2}, \sqrt{2}, i, -i\}$ for some 4×4 nonnegative matrix A. Then $\rho(A) = \sqrt{2}$, but since it is not an algebraically simple eigenvalue of A, the Perron-Frobenius Theorem implies A must be reducible. This implies $\{\sqrt{2}, i, -i\}$ must be the spectrum of a nonnegative matrix as well, but Theorem 3.1(d) fails for $k = 1$ and $m = 2$, since $s_1 = \sqrt{2}$ and $s_2 = 0$.*

An important additional necessary condition for the NIEP, known as Karpelevich's Theorem, which is independent of those outlined in Theorem 3.1, follows from the equivalence of the general NIEP with the *stochastic NIEP* (StNIEP). This equivalence was first established by Johnson [15], and is what we describe next. In particular, suppose $A \geq 0$ is an irreducible $n \times n$ matrix with $\sigma = \{\lambda_1, \lambda_2, \dots, \lambda_n\}$, and $\rho(A) = \lambda_1 > 0$. Let $x = [x_1, x_2, \dots, x_n]^T \gg 0$ be the positive eigenvector of A corresponding to λ_1. Now, let $D = \mathrm{diag}(x_1, x_2, \dots, x_n)$, and consider the matrix $B = \frac{1}{\lambda_1} D^{-1} A D \geq 0$. If we let $e = [1, 1, \dots, 1]^T$ be the $n \times 1$ vector of ones, we have:

$$Be = \frac{1}{\lambda_1} D^{-1} A D e = \frac{1}{\lambda_1} D^{-1} A x = \frac{1}{\lambda_1} D^{-1} \lambda_1 x = D^{-1} x = e.$$

That is, B is a stochastic matrix with spectrum $\sigma(B) = \frac{1}{\lambda_1}\sigma(A)$, and A and B are (diagonally) similar.

In case A is reducible, suppose A is in Frobenius normal form as follows:

$$A = \begin{bmatrix} A_{11} & 0 & \cdots & 0 \\ A_{21} & A_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \cdots & A_{mm} \end{bmatrix}$$

where each A_{ii} is $n_i \times n_i$ and irreducible, and $n_1 + n_2 + \cdots + n_m = n$. Then $\sigma(A)$ is the union of the $\sigma(A_{ii})$'s, and suppose each $\sigma(A_{ii})$ has spectral radius $\lambda_i > 0$ (with $\lambda_i \le \lambda_1$). Select $x^{(i)} \gg 0$ and define the matrix $D_i = \operatorname{diag}(x_1^{(i)}, x_2^{(i)}, \ldots, x_{n_i}^{(i)})$. Observe then that $D_i^{-1}A_{ii}D_i e = \lambda_i e$ (for e $n_i \times n_i$). Hence, letting $B_{i1} \ge 0$ be an arbitrary $n_{i+1} \times n_i$ matrix with row sums equal to $1 - \frac{\lambda_i}{\lambda_1}$, if we define:

$$B = \begin{bmatrix} \frac{1}{\lambda_1}D_1^{-1}A_{11}D_1 & 0 & \cdots & 0 \\ B_{21} & \frac{1}{\lambda_1}D_2^{-1}A_{22}D_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ B_{m1} & 0 & \cdots & \frac{1}{\lambda_1}D_m^{-1}A_{mm}D_m \end{bmatrix},$$

it follows that $Be = e$ and $\sigma(B) = \frac{1}{\lambda_1}\sigma(A)$ as before (only now A and B are not similar).

Let $\Theta_n \subset \mathbb{C}$ be the set of all eigenvalues of $n \times n$ stochastic matrices. That is, λ is an eigenvalue of an $n \times n$ stochastic matrix if and only if $\lambda \in \Theta_n$. Our next result is a complete characterization of Θ_n, specifically, the boundary of Θ_n, and is due to Karpelevich [16]. See also [23, Chapter 7] for several useful examples and additional information regarding the result. Our somewhat shorter statement is due to Ito [14].

Theorem 3.3 (**Karpelevich's Theorem** [14]) *The region Θ_n is symmetric relative to the real axis, is included in the unit disc $|z| \leq 1$, and intersects the circle $|z| = 1$ at points $e^{2\pi i a/b}$, where a and b run over the relatively prime integers satisfying $0 \leq a \leq b \leq n$. The boundary of Θ_n consists of these points and of curvilinear arcs connecting them in circular order.*

Let the endpoints of an arc be $e^{2\pi i a_1/b_1}$ and $e^{2\pi i a_2/b_2}$ ($b_1 \leq b_2$). Each of these arcs is given by the following parametric equation:

$$\lambda^{b_2}(\lambda^{b_1} - s)^{[n/b_1]} = (1-s)^{[n/b_1]}\lambda^{b_1[n/b_1]}, \tag{3.2}$$

where $[p/q]$ is the largest integer less than p/q, and the real parameter s runs over the interval $0 \leq s \leq 1$.

We note that the previous two results are useful for proving that a given list σ is not the spectrum of a nonnegative matrix, but cannot in general allow one to conclude for certain that a list is the spectrum of a nonnegative matrix.

In the next two examples, and since we require them for our work later, we illustrate Karpelevich's Theorem by constructing Θ_n for $n = 3, 4$ (see Figure 1). Note that $\Theta_n \subset \Theta_{n+1}$, since to any stochastic $n \times n$ matrix we may append a row and column of zeros without changing the spectrum (except adding a 0 to it).

Example 3.4 *Let $n = 3$ in Karpelevich's Theorem. Θ_3 intersects the circle $|z| = 1$ at points $1, -1, e^{2\pi i/3}, e^{4\pi i/3}$. Since Θ_2 is the real interval $[-1, 1]$, the arc connecting 1 to -1 in Θ_3 is this interval. Consider the arc connecting $1, e^{2\pi i/3}$, where $a_1 = 0, b_1 = 1, a_2 = 1, b_2 = 3$. The resulting parametric equation (3.2) is:*

$$\lambda^3(\lambda - s)^3 = (1-s)^3\lambda^3,$$

for $0 \leq s \leq 1$. *The nonconstant solutions to the above are:*

$$\lambda = \frac{3s-1}{2} \pm i\sqrt{3}\left(\frac{1-s}{2}\right).$$

So, taking the positive root above yields the line segment connecting $1, e^{2\pi i/3}$*; the negative root yields that connecting* $1, e^{4\pi i/3}$.

Now,for $a_1 = 1, b_1 = 2, a_2 = 1, b_2 = 3$, *we have:*

$$\lambda^3(\lambda^2 - s) = (1-s)\lambda^2,$$

for $0 \leq s \leq 1$ *which has (nonconstant) solutions*

$$\lambda = -\frac{1}{2} \pm \frac{i}{2}\sqrt{4s-3}.$$

So, the arc connecting $e^{2\pi i/3}$ *and* -1 *consists of two parts, taking the negative root above: for* $0 \leq s \leq \frac{3}{4}$, *the line segment connecting points* $(-1, 0)$ *with* $(-1/2, 0)$, *and for* $\frac{3}{4} \leq s \leq 1$, *the line segment connecting* $(-1/2, 0)$ *with* $e^{2\pi i/3}$. *Taking the positive root yields the complex conjugate of these arcs, and determines those connecting* -1 *with* $e^{4\pi i/3}$.

Thus, Θ_3 *is the union of the real interval* $[-1, 1]$ *with the closed triangle with vertices* $1, e^{2\pi i/3}, e^{4\pi i/3}$. *See Figure 1(a).*

Example 3.5 *We now construct* Θ_4 *according to Karpelevich's Theorem. The boundary of* Θ_4 *intersects the unit disc at the points:* $1, e^{\pi i/2}, e^{2\pi i/3}, -1, e^{4\pi i/3}, e^{3\pi i/2}$.

For the arc connecting $1, e^{\pi i/2}$, *let* $a_1 = 0, b_1 = 1, a_2 = 1, b_2 = 4$. (3.2) *becomes:*

$$\lambda^4(\lambda - s)^4 = (1-s)^4\lambda^4,$$

for $0 \leq s \leq 1$. *The nonconstant solutions to the above are:* $\lambda = 2s - 1, s \pm i(1-s)$. *The latter solutions are line segments connecting* $1, e^{\pi i/2}$ *and* $1, e^{3\pi i/2}$, *respectively taking the* $+$ *and* $-$ *above.*

The arcs connecting $e^{\pi i/2}, e^{2\pi i/3}$ *requires* $a_1 = 1, b_1 = 3, a_2 = 1, b_2 = 4$, *so* (3.2) *becomes:*

$$\lambda^4(\lambda^3 - s) = (1-s)\lambda^3,$$

hence, factoring and eliminating constant solutions, we have:

$$(\lambda + 1)(\lambda^2 + 1) = s \tag{3.3}$$

for $0 \leq s \leq 1$. *Replacing* λ *with* $\bar{\lambda}$ *gives the arc connecting* $e^{4\pi i/3}$ *and* $e^{3\pi i/2}$. *Similarly, the arc connecting* $e^{2\pi i/3}, -1$ *requires* $a_1 = 1, b_1 = 2, a_2 = 1, b_2 = 3$, *hence* (3.2) *becomes:*

$$\lambda^3(\lambda^2 - s)^2 = (1-s)^2\lambda^4,$$

i.e.

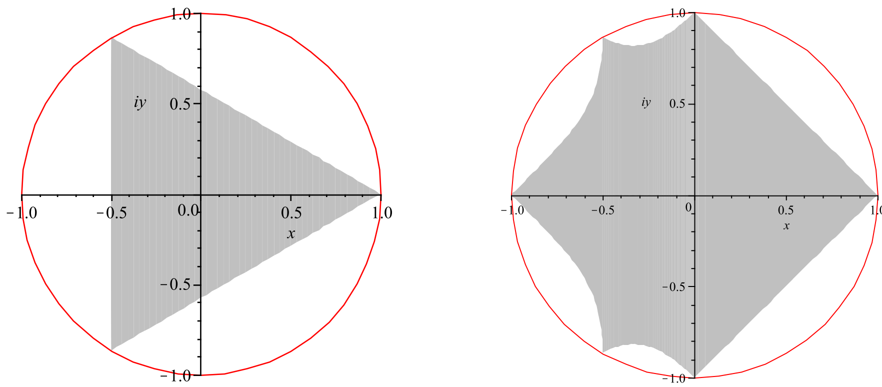
$$\lambda^4 - 2s\lambda^2 - (s^2 - 2s + 1)\lambda + s^2 = 0, \tag{3.4}$$

for $0 \leq s \leq 1$. *As before, replacing* λ *with* $\bar{\lambda}$ *yields the arc connecting* $-1, e^{4\pi i/3}$.

Now, the polynomials in (3.3), (3.4) *have a closed-form solution set as can be determined by Cardano's or Ferrari's Formulas; we do not present them here. They are easily plotted in Maple: see Figure 1(b).*

The regions Θ_n for $n = 3, 4$ are plotted below.

Remark 3.6 *In general, Karpelevich's Theorem is useful for providing bounds on the imaginary parts of individual complex numbers in the spectrum of a nonnegative matrix. However, if* σ *is a list of* $n \geq 5$ *complex numbers, and* $\lambda, \mu \in \Theta_n$ *are distinct, Karpelevich's Theorem does not imply that* λ *and* μ *are both eigenvalues of the same* $n \times n$ *nonnegative matrix. This is not the case if* λ, μ *are complex, nonreal numbers and* $n \leq 4$, *in which case* $\mu = \bar{\lambda}$.



(a) Θ_3 (b) Θ_4

Figure 1: The regions Θ_3 and Θ_4 as determined by Karpelevich's Theorem.

We now describe some sufficient conditions for the real NIEP (RNIEP) which lead to sufficient conditions for the NNIEP.

3.1.2 Some Sufficient Conditions for the RNIEP

In this section we present a few known sufficient conditions for the RNIEP, some of which date back to the inception of the problem. In the following we assume $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. Suleimanova [35] stated and Perfect [26] proved that if

$$\lambda_1 + \sum_{i,\lambda_i<0} \lambda_i \geq 0 \tag{3.5}$$

then $\sigma = \{\lambda_1, \lambda_2, \ldots, \lambda_n\}$ is the spectrum of an $n \times n$ (stochastic) nonnegative matrix. This result was improved by Salzmann [29], who found the following conditions sufficient for the existence of a diagonalizable nonnegative $n \times n$ matrix:

$$\begin{aligned} &\frac{1}{2}(\lambda_i + \lambda_{n+1-i}) \leq \frac{1}{n}\sum_{j=1}^{n} \lambda_j, \quad i = 2, \ldots, \left[\frac{n+1}{2}\right], \\ &\sum_{j=1}^{n} \lambda_j \geq 0 \end{aligned} \tag{3.6}$$

Salzmann's result was further refined by Kellogg [17] and later generalized by Fiedler [11] who deduced the existence of a nonnegative symmetric matrix with spectrum given as ordered above. In particular, let r be the greatest index j $(1 \leq j \leq n)$ for which $\lambda_j \geq 0$, and define:

$$K = \left\{ i \in \left\{ 1, 2, \ldots, \left[\frac{n-1}{2} \right] \right\} : \lambda_i \geq 0 \text{ and } \lambda_i + \lambda_{n-i} < 0 \right\}.$$

If

$$\begin{aligned} \lambda_1 + \sum_{\substack{i \in K \\ i < k}} (\lambda_i + \lambda_{n-i}) + \lambda_{n-k} \geq 0, &\quad \text{for all } k \in K, \\ \lambda_1 + \sum_{i \in K} (\lambda_i + \lambda_{n-i}) + \sum_{j=r+1}^{n-1-r} \lambda_j \geq 0, &\quad \text{provided } n \geq 2r+2, \end{aligned} \tag{3.7}$$

then σ is the spectrum of an $n \times n$ nonnegative matrix. Borobia [2] proved the following further generalization of Kellogg's condition (3.7). Define r as before to be the greatest index j $(1 \leq j \leq n)$ for which $\lambda_j \geq 0$, and let $J = \{\lambda_{r+1}, \ldots, \lambda_n\}$. If some partition $J_1 \cup \cdots \cup J_s$ of J exists such that the list:

$$\lambda_1 \geq \cdots \geq \lambda_r \geq \sum_{\lambda \in J_s} \lambda \geq \sum_{\lambda \in J_{s-1}} \lambda \geq \cdots \geq \sum_{\lambda \in J_1} \lambda \tag{3.8}$$

satisfies (3.7), then $\{\lambda_1, \lambda_2, \ldots, \lambda_n\}$ is the spectrum of a nonnegative matrix.

Remark 3.7 *Condition* (3.8) *is the most general of* (3.5)-(3.8). *That* (3.7) *implies* (3.8) *is obvious. Fiedler [11] and Marijuan, et. al [20] proved* (3.5) *and* (3.6) *imply* (3.8)*, and none of the converses are true since* $\sigma = \{5, 3, -2, -2, -2, -2\}$ *satisfies* (3.8) *but none of the rest. Also,* (3.5) *and* (3.6)*, and* (3.5) *and* (3.7) *are independent. To see this, let* $\sigma_1 = \{4, 3, -1, -2, -3\}$, $\sigma_2 = \{14, 6, 1, -7, -8\}$, $\sigma_3 = \{9, 7, 4, -3, -3, -6, -8\}$, *and* $\sigma_4 = \{3, 3, -1, -1. -2, -2\}$. *Then* σ_1 *satisfies* (3.5) *but not* (3.6) *and* σ_2 *satisfies*

(3.6) *but not* (3.5)*, while* σ_3 *satisfies* (3.5) *but not* (3.7) *and* σ_4 *satisfies* (3.7) *but not* (3.5).

We now proceed to the NNIEP.

3.2 Sufficient Conditions for NNIEP

In this section, we collect some sufficient conditions for the NNIEP. We include proofs only where short, or somewhat simple, or where no proof can be found in the literature. Practically all such known conditions are based on the existence or construction of *circulant* matrices, which have the form:

$$A = \begin{bmatrix} a_1 & a_2 & \cdots & a_n \\ a_n & a_1 & \cdots & a_{n-1} \\ \vdots & \vdots & \ddots & \vdots \\ a_2 & a_3 & \cdots & a_1 \end{bmatrix}.$$

Circulant matrices enjoy many nice properties (see [8]). In particular, they are normal, and if a nonnegative circulant matrix is scaled so that it's spectral radius is equal to 1, then it is doubly stochastic. Let $\sigma(A) = \{\lambda_1, \lambda_2, \ldots, \lambda_n\}$ and $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$. If U is the $n \times n$ normalized Fourier matrix, i.e.

$$U = \frac{1}{\sqrt{n}} \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & w_1 & w_1^2 & \cdots & w_1^{n-1} \\ \vdots & \vdots & \ddots & \vdots & \\ 1 & w_{n-1} & w_{n-1}^2 & \cdots & w_{n-1}^{n-1} \end{bmatrix}$$

where

$$w_i = e^{2\pi ik/n} = \cos\frac{2k\pi}{n} + i\sin\frac{2k\pi}{n}, \quad k = 1, \ldots, n,$$

then U is unitary, i.e. $UU^* = I$, and:

$$A = U\Lambda U^*.$$

The nonnegative inverse eigenvalue problem for circulant matrices has been solved by Rojo and Soto [28, Theorem 10], who proved the following.

Theorem 3.8 [28] *Let* $\sigma = \{\lambda_1, \lambda_2, \ldots, \lambda_n\}$ *be a list of complex numbers labeled so that*

(a) $\lambda_1 \geq \max_{2\leq k\leq n} |\lambda_k|$,

(b) $\lambda_{n-j+2} = \bar{\lambda}_j$ *for* $j = 2, 3, \ldots, \left[\frac{n+1}{2}\right]$.

Then σ *is the spectrum of a nonnegative* $n \times n$ *circulant matrix if and only if* λ_1 *is at least:*

$$\min_{p\in\mathscr{P}} \max_{0\leq k\leq 2m} \left\{ -2\sum_{j=2}^{m+1} \mathrm{Re}p(\lambda_j) \cos\frac{2k(j-1)\pi}{2m+1} - 2\sum_{j=2}^{m+1} \mathrm{Im}p(\lambda_j) \sin\frac{2k(j-1)\pi}{2m+1} \right\} \tag{3.9}$$

if $n = 2m+1$, *or*

$$\begin{aligned} \min_{p\in\mathscr{P}} \max_{0\leq k\leq 2m+1} \Bigg\{ -2\sum_{j=2}^{m+1} \mathrm{Re}p(\lambda_j) \cos\frac{k(j-1)\pi}{m+1} - (-1)^k\lambda_{m+2} \\ -2\sum_{j=2}^{m+1} \mathrm{Im}p(\lambda_j) \sin\frac{k(j-1)\pi}{m+1} \Bigg\} \end{aligned} \tag{3.10}$$

if $n = 2m+2$, *where*

$$\begin{aligned} \mathscr{P} = \{p : p \text{ permutation on } \{\lambda_2, \ldots, \lambda_n\}, \\ p(\lambda_j) = \lambda_k \text{ iff } p(\lambda_{n-j+2}) = \bar{\lambda}_k,\ j = 2, 3, \ldots, n\} \end{aligned} \tag{3.11}$$

The following corollary of Theorem 3.8, proved independently by Xu [37, Theorem 2.3], leads to additional results from which sufficient conditions for the more general NNIEP arise.

Corollary 3.9 [37] *Let* $\sigma = \{\lambda_1; \lambda_2, \ldots, \lambda_{m+1}, \bar{\lambda}_2, \ldots, \bar{\lambda}_{m+1}\}$ *and* $\mathrm{Im}\lambda_i \neq 0$ *for* $i = 2, \ldots, m+1$. *If*

$$\lambda_1 \geq 2(|\lambda_2| + \cdots + |\lambda_{m+1}|),$$

then there exists an $n \times n$ *nonnegative circulant matrix with spectrum* σ*, where* $n = 2m+1$.

Proof. Select $p \in \mathscr{P}$ as in (3.11), and suppose σ is relabeled if necessary in accordance with p, so that the first m complex λ_i's are the conjugates of the last m. Suppose $p(\lambda_j) = x_j + iy_j$, where $y_j \neq 0$, for $j = 2, \ldots, m+1$. A computation using (3.9) reveals:

$$\begin{aligned}
&\max_{0 \leq k \leq 2m} \left\{ -2 \sum_{j=2}^{m+1} \mathrm{Re}p(\lambda_j) \cos \frac{2k(j-1)\pi}{2m+1} - 2 \sum_{j=2}^{m+1} \mathrm{Im}p(\lambda_j) \sin \frac{2k(j-1)\pi}{2m+1} \right\} \\
&= -2 \sum_{j=2}^{m+1} \sqrt{x_j^2 + y_j^2} \left(\frac{x_j}{\sqrt{x_j^2 + y_j^2}} \cos \frac{2k^*(j-1)\pi}{2m+1} + \frac{y_j}{\sqrt{x_j^2 + y_j^2}} \sin \frac{2k^*(j-1)\pi}{2m+1} \right) \\
&\leq 2 \sum_{j=2}^{m+1} |p(\lambda_j)| \cdot \left| \frac{x_j}{\sqrt{x_j^2 + y_j^2}} \cos \frac{2k^*(j-1)\pi}{2m+1} + \frac{y_j}{\sqrt{x_j^2 + y_j^2}} \sin \frac{2k^*(j-1)\pi}{2m+1} \right| \\
&\leq 2 \sum_{j=2}^{m+1} |p(\lambda_j)| \\
&= 2(|\lambda_2| + \cdots + |\lambda_{m+1}|) \\
&\leq \lambda_1.
\end{aligned}$$

Appealing to Theorem 3.8 yields the result. □

The following interesting result, found in Fiedler [11, Lemma 2.2] and generalized by Xu [37, Lemma 2.4], is used to construct additional normal matrices, which may not be circulants, from two given normal matrices. The proof is based on direct construction, and so we omit it.

Theorem 3.10 [37] *Let A be an $m \times m$ normal matrix with eigenvalues $\alpha_1, \ldots, \alpha_m$, let u, $\|u\| = 1$, be an eigenvector corresponding to α_1; let B be an $n \times n$ normal matrix with eigenvalues $\beta_1, \ldots, \beta_n$, let v, $\|v\| = 1$, be an eigenvector corresponding to β_1, then for any ρ, the matrix*

$$C = \begin{bmatrix} A & \rho u v^* \\ \rho v u^* & B \end{bmatrix}$$

has eigenvalues $\alpha_2, \ldots, \alpha_m, \beta_2, \ldots, \beta_n, \nu_1, \nu_2$, where ν_1 and ν_2 are eigenvalues of the matrix

$$\hat{C} = \begin{bmatrix} \alpha_1 & \rho \\ \rho & \beta_1 \end{bmatrix}.$$

Remark 3.11 *If $A \geq 0$ and $B \geq 0$ in Theorem (3.10), the Perron-Frobenius Theorem implies both u and v are nonnegative, hence $C \geq 0$ as well.*

Notice that the selection of ρ, in addition to the matrices A and B, completely determines ν_1 and ν_2, as well as the matrix C, above. By selecting ρ properly, one can construct a new nonnegative normal matrix from two nonnegative normal matrices, altering only the respective spectral radii of the original matrices [37, Theorem 2.5].

Theorem 3.12 [37] *If $\{\alpha_0; \alpha_1, \ldots, \alpha_{m-1}\}$ and $\{\beta_0; \beta_1, \ldots, \beta_{n-1}\}$ are the spectra of nonnegative normal matrices $A \in M_m$ and $B \in M_n$ respectively, and $\alpha_0 \geq \beta_0$, then for any $\eta \geq 0$,*

$$\{\alpha_0 + \eta; \beta_0 - \eta, \alpha_1, \ldots, \alpha_{m-1}, \beta_1, \ldots, \beta_{n-1}\}$$

is the spectrum of a nonnegative normal matrix $C \in M_{m+n}$.

Proof. Take $\rho = \sqrt{\eta(\alpha_0 + \beta_0 + \eta)}$ in Theorem 3.10. Clearly $C \geq 0$; that C is also normal follows since C has an orthonormal set of $m + n$ eigenvectors. □

Theorems 3.9 and 3.12 together imply the following more general result [37, Corollary 2.7].

Theorem 3.13 [37] *Let* $\sigma = \{\lambda_0 1; \lambda_1, \ldots, \lambda_t, \lambda_{t+1}, \ldots, \lambda_s, \mu_1, \ldots, \mu_m, \bar{\mu}_1, \ldots, \bar{\mu}_m\}$ *where* $\lambda_0 \geq \lambda_1 \geq \cdots \geq \lambda_t \geq 0 \geq \lambda_{t+1} \geq \cdots \geq \lambda_s$ *are real and* $\mathrm{Im}\mu_k \neq 0$ *for* $k = 1, \ldots, m$. *If*

$$\lambda_o \geq |\lambda_{t+1}| + \cdots + |\lambda_s| + 2|\mu_1| + \cdots + 2|\mu_m|,$$

then there exists an $n \times n$ *normal nonnegative matrix with spectrum* σ*, where* $n = 2m + s + 1$.

Proof. We first prove the case $t = 0$. Here we proceed by induction on s. If $s = 0$, the assertion follows from Theorem 3.9. If $s = 1$, let $\lambda_0' = \lambda_0 + \lambda_1$ and $\lambda_1' = 0$. Theorem We first prove the case $t = 0$. Here we proceed by induction on s. If $s = 0$, the assertion follows from Theorem 3.9 implies there is a $(2m+1) \times (2m+1)$ nonnegative circulant matrix with spectrum $\{\lambda_0'; \mu_1, \ldots, \mu_m, \bar{\mu}_1, \ldots, \bar{\mu}_m\}$. Since $[0]$ is normal, applying Theorem 3.12 with $\eta = |\lambda_1|$ yields that

$$\{\lambda_0; \lambda_1, \mu_1, \ldots, \mu_m, \bar{\mu}_1, \ldots, \bar{\mu}_m\}$$

is the spectrum of a $2m + 2$ nonnegative normal matrix.

Suppose the result is true for all $k \leq s$ where $s \geq 2$. Let $\lambda_0' = \lambda_0 + \lambda_1$, $\lambda_1' = \lambda_2, \ldots, \lambda_{s-1}' = \lambda_s$. By the induction hypothesis, there exists a nonnegative normal $(2m + s) \times (2m + s)$ matrix with spectrum $\{\lambda_0'; \lambda_1', \ldots, \lambda_{s-1}', \mu_1, \ldots, \mu_m, \bar{\mu}_1, \ldots, \bar{\mu}_m\}$. Again, since $[0]$ is normal, we apply Theorem 3.12 with $\eta = |\lambda_1|$ to obtain that

$$\{\lambda_0; \lambda_1, \lambda_2, \ldots, \lambda_s, \mu_1, \ldots, \mu_m, \bar{\mu}_1, \ldots, \bar{\mu}_m\}$$

is the spectrum of a nonnegative normal $(2m+s+1)\times(2m+s+1)$ matrix. This completes the induction and proves the case $t=0$.

Now, if $t \geq 1$, we take the direct sum of the aforementioned $(2m+s+1)\times(2m+s+1)$ matrix with the (nonnegative, normal) diagonal matrix $\mathrm{diag}(\lambda_1,\ldots,\lambda_t)$ and obtain a nonnegative normal matrix with desired spectrum. This completes the proof. $\square$

We now turn to the comparison of sufficient conditions for the RNIEP with those for the NNIEP. To do so, we require some further definitions as found in [37]. For a $(2m+s+1)$-tuple of complex numbers

$$\sigma = \{\lambda_0; \lambda_1, \ldots, \lambda_s, \mu_1, \ldots, \mu_m, \bar{\mu}_1, \ldots, \bar{\mu}_m\}, \tag{3.12}$$

where $\lambda_0, \lambda_1, \ldots, \lambda_s$ are real, $\lambda_0 \geq 0$, and $\mathrm{Im}\mu_j \neq 0$ $(0 \leq j \leq m)$, we define:

$$\begin{gathered} r_o' = \lambda_0, \quad r_i' = \lambda_i \quad (1 \leq i \leq s), \\ r_{s+j}' = -2|\mu_j| \quad (1 \leq j \leq m) \end{gathered} \tag{3.13}$$

We call the set

$$\sigma' = \{r_0'; r_1', \ldots, r_s', r_{s+1}', \ldots, r_{s+m}'\} \tag{3.14}$$

the *companion set* of σ. Note σ' is a $(s+m+1)$-tuple of real numbers.

Observe that Theorem 3.13 shows that if the companion set of σ satisfies Perfect's sufficient condition (3.5), then there is a nonnegative normal matrix with spectrum σ. That this is also true for Salzmann's and Kellogg's conditions (3.6), (3.7) is proved in [37, Corollary 2.9, Theorem 2.8]. We state the results here for completeness, but omit the rather lengthy proofs.

Theorem 3.14 [37] *Let σ and σ' be given by* (3.12) *and* (3.13), *respectively, and σ' be ordered as $r_0 \geq r_1 \geq \cdots \geq r_n$, where $n = s+m$ and $r_i = r'_{\tau(i)}, (0 \leq i \leq n)$ for some* *permutation τ. If*

$$\frac{1}{2}(r_i + r_{n-i}) \leq \frac{1}{n+1}\sum_{j=0}^{n} r_j, \quad i = 1, \ldots, \left[\frac{n}{2}\right],$$

$$\sum_{i=0}^{n} r_i \geq 0,$$

then there exists a normal nonnegative matrix with spectrum σ.

Theorem 3.15 [37] *Let σ and σ' be given by* (3.12) *and* (3.13)*, respectively, and σ' be ordered as $r_0 \geq r_1 \geq \cdots \geq r_n$, where $n = s + m$ and $r_i = r'_{\tau(i)}, (0 \leq i \leq n)$ for some permutation τ. Let*

$$K = \left\{ i \in \left\{1, \ldots, \left[\frac{n}{2}\right]\right\} : r_i \geq 0 \text{ and } r_i + r_{n+1-i} < 0 \right\}$$

and q be the greatest index j $(0 \leq j \leq n)$ for which $r_j \geq 0$. If

$$r_0 + \sum_{\substack{i \in K \\ i < k}} (r_i + r_{n+1-i}) + r_{n+1-k} \geq 0 \quad \text{for all } k \in K,$$

$$r_0 + \sum_{i \in K} (r_i + r_{n+1-i}) + \sum_{j=q+1}^{n-q} r_j \geq 0,$$

then there exists a $(2m+s+1) \times (2m+s+1)$ normal nonnegative matrix with spectrum σ.

Finally, it was proved by Radwan [27, Theorem 3.3] that if a certain set derived from the companion set of σ satisfies Kellogg's condition (3.7), then we obtain a sufficient condition for the existence of a nonnegative normal matrix that is similar in generality to that of Borobia's (3.8). We state Radwan's conditions without proof as we conclude this section.

Theorem 3.16 [27] *Let $\sigma = \{\lambda_0, \lambda_1, \ldots, \lambda_l, \mu_1, \ldots, \mu_m, \bar{\mu}_1, \ldots, \bar{\mu}_m\}$ where $\lambda_0 \geq \lambda_1 \geq \cdots \geq \lambda_l$ are real numbers, $\lambda_0 \geq 0$, and $\mathrm{Im}\mu_j \neq 0$ for all $j = 1, 2, \ldots, m$. Let $\sigma' = \{r_0, r_1, \ldots, r_{l+m}\}$ be the companion set of σ, arranged so that $r_0 \geq r_1 \geq \cdots \geq r_{l+m}$. Let q be the greatest index j $(0 \leq j \leq l)$ for which $r_j \geq 0$. Let S be an integer such that $1 \leq S \leq l+m-q$, and let $J_1 \cup J_2 \cup \cdots \cup J_S$ be an S-partition of $J = \{-r_{q+1}, -r_{q+2}, \ldots, -r_{l+m}\}$ where*

$$\sum_{r \in J_1} r \geq \sum_{r \in J_2} r \geq \cdots \geq \sum_{r \in J_S} r.$$

Define $T_j = \sum_{J_j} r$, $j = 1, 2, \ldots, S$.

If $\{r_0, r_1, \ldots, r_q, -T_S, -T_{S-1}, \ldots, -T_1\}$ satisfies Kellogg's condition (3.7), then σ is the spectrum of a nonnegative normal $(2m+l+1) \times (2m+l+1)$ matrix.

As a final remark, we consider the following example.

Example 3.17 *Let $\sigma = \{12\sqrt{2}, -12, 12+i, 12-i\}$. Observe that the companion set of σ is $\sigma' = \{12\sqrt{2}, -12, -2\sqrt{145}\}$, which is not the spectrum of any 3×3 nonnegative matrix since the sum of its entries is negative. Indeed, σ does not satisfy any of the sufficient conditions stated in this section to be the spectrum of a nonnegative normal 4×4 matrix. In particular, σ is not the spectrum of a 4×4 nonnegative circulant matrix. However, σ is the spectrum of the following nonnegative normal 4×4 matrix:*

$$A = 12\sqrt{2}\begin{bmatrix} \frac{1}{6} - \frac{\sqrt{2}}{12} & \frac{1}{6} + \frac{5\sqrt{2}}{12} & \frac{\sqrt{2}}{6} - \frac{1}{6} - \frac{\sqrt{3}}{72} & \frac{\sqrt{2}}{6} - \frac{1}{6} + \frac{\sqrt{3}}{72} \\ \frac{1}{6} + \frac{5\sqrt{2}}{12} & \frac{1}{6} - \frac{\sqrt{2}}{12} & \frac{\sqrt{2}}{6} - \frac{1}{6} - \frac{\sqrt{3}}{72} & \frac{\sqrt{2}}{6} - \frac{1}{6} + \frac{\sqrt{3}}{72} \\ \frac{\sqrt{2}}{6} - \frac{1}{6} + \frac{\sqrt{3}}{72} & \frac{\sqrt{2}}{6} - \frac{1}{6} + \frac{\sqrt{3}}{72} & \frac{1}{3} + \frac{\sqrt{2}}{3} & \frac{1}{3} - \frac{\sqrt{2}}{6} - \frac{\sqrt{6}}{72} \\ \frac{\sqrt{2}}{6} - \frac{1}{6} - \frac{\sqrt{3}}{72} & \frac{\sqrt{2}}{6} - \frac{1}{6} + \frac{\sqrt{3}}{72} & \frac{1}{3} - \frac{\sqrt{2}}{6} + \frac{\sqrt{6}}{72} & \frac{1}{3} + \frac{\sqrt{2}}{3} \end{bmatrix}.$$

The means by which we construct A, namely the matrix S in Case 2 of Section 3.3.2 *with quasi-diagonal form:*

$$\Lambda = \begin{bmatrix} 12\sqrt{2} & 0 & 0 & 0 \\ 0 & 12 & 1 & 0 \\ 0 & -1 & 12 & \\ 0 & 0 & 0 & -12 \end{bmatrix},$$

will be discussed in the next section.

3.3 Skew-Symmetric Sign Patterns Allowing Positive Null Vectors

Recall that if N is an $n \times n$ normal matrix, then $N = S + K$ where $S = S^T$ is symmetric and $K = -K^T$ is skew-symmetric, each of S and K are also normal, hence possess a common orthonormal set of n eigenvectors. Now, suppose $N \geq 0$, and

$$\sigma(N) = \{\lambda_1, \ldots, \lambda_s, \alpha_1 + i\beta_1, \ldots, \alpha_m + i\beta_m, \alpha_1 - i\beta_1, \ldots, \alpha_m - i\beta_m\},$$

where $\lambda_1 \geq 0$, $\lambda_k \in \mathbb{R}$ $(1 \leq k \leq s)$ and $\beta_j > 0$ $(i \leq j \leq m)$. Then $S \geq 0$ as well, and

$$\sigma(S) = \{\lambda_1, \ldots, \lambda_s, \alpha_1, \ldots, \alpha_m, \alpha_1, \ldots, \alpha_m\}$$

and

$$\sigma(K) = \{\underbrace{0, \ldots, 0}_{s \text{ terms}}, i\beta_1, \ldots, i\beta_m, -i\beta_1, \ldots, -i\beta_m\}.$$

If $\rho(N) = \lambda_1 \geq 0$, N has a nonnegative eigenvector corresponding to λ_1 which thus corresponds to λ_1 for S and to 0 for K. That is, K must have a nonnegative null vector. If N is also irreducible, it follows that K must have a positive null vector.

In order for K to have a positive null vector, there are certain restrictions that must be placed on its sign pattern which, in turn, place restrictions on the orthonormal set of eigenvectors of K, S, and thus N. The analysis of the prevailing sign patterns leads to a method for solving the NNIEP which shows promise. Specifically, we construct an orthonormal basis of eigenvectors of K, determine if $\sigma(S)$ is the set of eigenvalues of a nonnegative symmetric matrix S with the same eigenvector basis, and then see if $N = S+K \geq 0$ (the sum $S+K$ is then a normal matrix since S and K are simultaneously diagonalizable by construction).

We begin with a basic result characterizing skew-symmetric matrices from which our main results will follow, whose proof can be found in [13, Chapter 2].

Theorem 3.18 *Let K be an $n \times n$ skew-symmetric matrix. Then:*

(a) K is normal, hence there is a unitary matrix U such that U^*KU is a diagonal matrix.

(b) The eigenvalues of K are either 0 or pure imaginary numbers occurring in complex conjugate pairs.

(c) K has even rank, and the parity of n and the number of zero eigenvalues are the same. Thus if n is odd, then K is singular.

We are concerned here with sign patterns of skew-symmetric matrices, henceforth called *skew patterns*. As we shall see, skew patterns are relatively special, and form a proper subset of all sign-singular skew patterns.

Since our principal aim is directed toward sign patterns of null vectors, and transposition and permutation similarity do not effect positive such vectors, we make the following observation.

Observation 3.19 *The set of $n \times n$ skew patterns is closed under*

(a) permutation similarity, and

(b) transposition, i.e. multiplication by -1.

In view of the above result, there is no loss of generality in replacing $+$ and $-$ in a skew pattern with 1 and -1, each of the patterns considered below may be viewed as $\{1, -1, 0\}-$matrices rather than sign patterns.

Remark 3.20 *The set of $n \times n$ skew patterns is also closed under signature similarity: if K is a skew pattern and D is a diagonal matrix with 1's and -1's on its diagonal (i.e. a signature matrix), then DKD is also a skew pattern. However, signature similarity does not preserve positivity of null vectors, and so will not be included in the discussion here.*

We say that two skew patterns A and B are *equivalent* if B can be obtained from A by finitely many operations in Observation 3.19, and hence, this defines an equivalence relation. Consequently, to achieve our aforementioned goal, it suffices to consider representatives of equivalence classes.

We require now a, preferably simple, condition for determining whether or not a skew pattern allows a positive null vector. It is clear that a skew pattern with a positive null vector cannot have a row (or column) whose nonzero entries are all of the same sign: that is, each row must be multi-signed. The following lemma provides a necessary condition that is easy to check.

Lemma 3.21 *Let $K = [k_{ij}]$ be an $n \times n$ singular skew-symmetric matrix. If K has a* *positive null vector, then*

$$\left|\sum_{j=1}^{n} k_{ij}\right| \leq \sum_{j=1}^{n} |k_{ij}|, \quad i = 1, \ldots, n \tag{3.15}$$

with equality for some i *if and only if* $k_{ij} = 0$ *for all* $j = 1, \ldots, n$. *An analogous inequality also holds for the columns of* K.

Proof. By the triangle inequality for real numbers, if equality holds in (3.15) for some nonzero row (column) of K, then each nonzero entry of this row (column) must have the same sign, hence K cannot have a positive null vector. □

For $n = 3, 4$, and 5, Lemma 3.21 is also sufficient as a characterization of possible skew patterns as can be verified directly using the function `skewsp` implemented in MATLAB (see Appendix A.2). However, beginning with $n = 6$, the condition is not sufficient, as we now illustrate.

Example 3.22 *Let*

$$K = \begin{bmatrix} 0 & + & - & + & + & + \\ - & 0 & + & + & + & + \\ + & - & 0 & + & + & + \\ - & - & - & 0 & - & + \\ - & - & - & + & 0 & - \\ - & - & - & - & + & 0 \end{bmatrix}$$

Clearly K *satisfies* (3.15). *However,* K *does not possess a positive null vector. Let* K *have a positive null vector* $x = [x_1, \ldots, x_6]^T$. *Then* $Kx = 0$ *if and only if* $\hat{K}e = D^{-1}KDe = 0$ *where* $e = [1, \ldots, 1]^T \in \mathbb{R}^6$ *and* $D = \mathrm{diag}(x_1, \ldots, x_6)$ *(we used the same* *idea to prove the equivalence of the NIEP and the StNIEP in Section 3.1). Observe that* $\hat{K}$ *and* K *have the same sign pattern, only now the rows of* $\hat{K}$ *sum to* 0*. Suppose*

$$\hat{K} = \begin{bmatrix} 0 & a & -b & c & d & e \\ -a & 0 & f & g & h & j \\ b & -f & 0 & k & l & m \\ -c & -g & -k & 0 & -p & q \\ -d & -h & -l & p & 0 & -r \\ -e & -j & -m & -q & r & 0 \end{bmatrix},$$

where $a, b, c, d, e, f, g, h, j, k, l, m, p, q$ *are positive numbers.* $\hat{K}e = 0$ *implies the following three equations must hold:*

$$a = f + g + h + j$$

$$b = a + c + d + e$$

$$f = b + j + k + l.$$

Substituting the second equation for b *in the third equation, then substituting the resulting expression for* f *into the first equation yields:*

$$a = a + c + d + e + j + k + l + g + h + j,$$

hence $c + d + e + j + k + l + g + h + j = 0$*. This contradicts that the terms involved are positive. Therefore, no realization of the sign pattern* K *has a positive null vector.*

Let K be skew-symmetric and write $K = K_+ - K_+^T$ where $K_+ \geq 0$, the *positive part of* K, has nonzero entries only at indices where K is positive. Through an analysis of K_+, we obtain necessary and sufficient conditions for a skew-symmetric pattern to have a positive null vector, as follows.

Theorem 3.23 *Let $K \neq 0$ be a singular skew-symmetric pattern, and K_+ its positive part. Then K allows a positive null vector if and only if K_+ is irreducible, or the Frobenius normal form of K_+ is a direct sum of irreducible matrices.*

Proof. It suffices to prove the "if" part in the case that K_+ is irreducible. Hence the graph G of K_+ is strongly connected, and so each member of $E(G)$ belongs to some cycle. Assume that G contains p edge-distinct cycles. Then we may decompose the pattern K_+ as a sum of p cycle patterns $Z_1, Z_2, \ldots, Z_p$. Denote by $\hat{Z}_i$ the $\{0,1\}$-matrix obtained from Z_i by replacing $+$ with 1. By definition of cycle pattern, we see that the sum of each nonzero row and column of $\hat{Z}_i - \hat{Z}_i^T$ is 0, hence defining $\hat{K}_+$ as the sum of $\hat{Z}_1, \hat{Z}_2, \ldots, \hat{Z}_p$, we see that the skew-symmetric matrix $\hat{K} = \hat{K}_+ - \hat{K}_+^T$, satisfies:

$$\hat{K}e = \sum_{i=1}^{p} (\hat{Z}_i - \hat{Z}_i^T)e = \sum_{i=1}^{p} 0 = 0.$$

We have thus constructed a realization of the pattern K which has a positive null vector.

We shall prove the contrapositive of the "only if" part. Assume K is a singular skew-symmetric matrix with a reducible K_+, and that the Frobenius normal form of K_+ is not a direct sum. Without losing generality, we assume K_+ has the form:

$$\begin{bmatrix} K_1 & K_3 \\ 0 & K_2 \end{bmatrix}$$

where K_1 and K_2 are square nonnegative matrices, and K_3 is nonnegative and nonzero. Let x be a null vector of K, and partition $x = [x_1, x_2]^T$ to conform with K_+. Then:

$$Kx = \begin{bmatrix} (K_1 - K_1^T)x_1 & K_3 x_2 \\ -K_3^T x_1 & (K_2 - K_2^T)x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

Since $x_1^T(K_1 - K_1^T)x_1 = x_2^T(K_2 - K_2^T)x_2 = 0$ for any x_1, x_2, and $x^T K x = 0$, it follows that $x_1^T K_3 x_2 = 0$. So, x_1 or x_2 must contain at least one nonpositive entry, and thus cannot both be positive. Consequently, K cannot have a positive null vector, and this completes the proof. □

We have the following immediate corollary to Theorem 3.23.

Corollary 3.24 *Let K be a skew-symmetric pattern. The following are equivalent:*

(a) K allows a null vector with no zero entries;

(b) DKD allows a positive null vector for some signature matrix D;

(c) the positive part of DKD is irreducible, or its Frobenius normal form is a direct sum of irreducible matrices, for some signature matrix D.

We now proceed to the NNIEP for $n = 3$ and 4. Note that the SNIEP has been solved for $n = 3, 4$ by McDonald and Neumann [21], who used Soules matrices to construct solution matrices. For this reason, we focus our attention on the nonsymmetric NNIEP.

3.3.1 The NNIEP for 3×3 Matrices

We begin our exposition of the NNIEP for $n = 3$ with the following observation.

Observation 3.25 *There is only one equivalence class of 3×3 skew-symmetric matrices which allow a positive null vector and satisfy* (3.15). *This class is represented by the following sign-pattern matrix:*

$$\begin{bmatrix} 0 & + & - \\ - & 0 & + \\ + & - & 0 \end{bmatrix}.$$

Proof. The only two patterns which satisfy (3.15) and allow a positive null vector are

$$\begin{bmatrix} 0 & + & - \\ - & 0 & + \\ + & - & 0 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 0 & - & + \\ + & 0 & - \\ - & + & 0 \end{bmatrix}$$

and the first pattern is the transpose of the second. As an example, the null space of

$$\begin{bmatrix} 0 & 1 & -1 \\ -1 & 0 & 1 \\ 1 & -1 & 0 \end{bmatrix}$$

is spanned by $[1, 1, 1]^T$. □

We will now characterize the spectra of all 3×3 (nonsymmetric) normal matrices in terms of the nonzero entries of their skew-symmetric parts with sign patterns in accordance with Observation 3.25.

Theorem 3.26 *Let $A \geq 0$ be a (nonsymmetric) normal 3×3 matrix with $\sigma(A) = \{1, a + bi, a - bi\}$ $(b > 0)$ and unit Perron vector $\nu = [x, y, z]^T \gg 0$, where $x \geq y \geq z$. Then*

$$-\frac{z^2}{x^2 + y^2} \leq a \leq 1 \quad \text{and} \quad b \leq \frac{yz(1-a)}{x}. \tag{3.16}$$

Conversely, if $\sigma = \{1, a + bi, a - bi\}$ $(b > 0)$ and

$$-\frac{1}{2} \leq a \leq 1 \quad \text{and} \quad b \leq \frac{1-a}{\sqrt{3}} \tag{3.17}$$

are satisfied, there exists a nonnegative normal matrix with spectrum σ.

Before proceeding to the proof of Theorem 3.26, we make the following remark.

Remark 3.27 *Observe that conditions* (3.17) *are simply those of Theorem 3.1(c) and (d) adapted for* $\sigma = \{1, a+bi, a-bi\}$*, and* (3.17) *follows from* (3.16) *by taking* $x = y = z = \frac{1}{\sqrt{3}}$*. Also, the set* Θ_3 *constructed in Figure* 1*(a) is precisely the set obtained by graphing* (3.17)*. While* (3.17) *are thus sufficient for the existence of some normal matrix with the given spectrum, the first part of Theorem 3.26 indicates that the sharper inequalities* (3.16) *must hold for a given normal matrix with Perron vector* ν*.*

Proof of Theorem 3.26. Let $K = \frac{1}{2}(A - A^T)$ be the skew-symmetric part of A, and denote by $\hat{K}$ the matrix:

$$\hat{K} = \begin{bmatrix} 0 & z & -y \\ -z & 0 & x \\ y & -x & 0 \end{bmatrix}.$$

Note that $\sigma(\hat{K}) = \{0, i, -i\}$, and $\nu = [x, y, z]^T$ is a (positive) null vector of $\hat{K}$. By Observation 3.25, we may assume without losing generality that $K = b\hat{K}$, so that K and $\hat{K}$ are simultaneously unitarily diagonalizable. An invertible matrix diagonalizing $\hat{K}$ is:

$$R = \begin{bmatrix} x & \dfrac{-xz + iy}{x^2 + y^2} & \dfrac{-xz - iy}{x^2 + y^2} \\ y & \dfrac{-yz - ix}{x^2 + y^2} & \dfrac{-yz + ix}{x^2 + y^2} \\ z & 1 & 1 \end{bmatrix}.$$

Since R is not unitary, we apply the Gram-Schmidt procedure to R to obtain:

$$U = \begin{bmatrix} x & \dfrac{-xz + iy}{\sqrt{2(x^2 + y^2)}} & \dfrac{-xz - iy}{\sqrt{2(x^2 + y^2)}} \\ y & \dfrac{-yz - ix}{\sqrt{2(x^2 + y^2)}} & \dfrac{-yz + ix}{\sqrt{2(x^2 + y^2)}} \\ z & \sqrt{\dfrac{x^2 + y^2}{2}} & \sqrt{\dfrac{x^2 + y^2}{2}} \end{bmatrix}.$$

Now, U not only diagonalizes $\hat{K}$ and K, but also A itself, hence letting $\Lambda = \mathrm{diag}(1, a+bi, a-bi)$, it follows that:

$$A = U\Lambda U^* = \begin{bmatrix} x^2+(y^2+z^2)a & xy(1-a)+zb & xz(1-a)-yb \\ xy(1-a)-zb & y^2+(x^2+z^2)a & yz(1-a)+xb \\ xz(1-a)+yb & yz(1-a)-xb & z^2+(x^2+y^2)a \end{bmatrix}. \tag{3.18}$$

So, $A \geq 0$ if and only if the following inequalities are satisfied:

$$-\min\left\{\frac{x^2}{y^2+z^2}, \frac{y^2}{x^2+z^2}, \frac{z^2}{x^2+y^2}\right\} \leq a \leq 1,$$

and

$$b \leq \min\left\{\frac{xy(1-a)}{z}, \frac{xz(1-a)}{y}, \frac{yz(1-a)}{x}\right\}.$$

By our assumption that $x \geq y \geq z$, we have $x^2 \geq y^2 \geq z^2$ and $x^2+y^2 \geq x^2+z^2 \geq y^2+z^2$, and also $xy \geq xz \geq zy$. Therefore,

$$\frac{x^2}{y^2+z^2} \geq \frac{y^2}{x^2+z^2} \geq \frac{z^2}{x^2+y^2} \quad \text{and} \quad \frac{xy(1-a)}{z} \geq \frac{xz(1-a)}{y} \geq \frac{yz(1-a)}{x},$$

hence (3.16) holds.

To prove (3.17), it suffices to take $x = y = z = \frac{1}{\sqrt{3}}$ in (3.18). This completes the proof. $\square$

As a corollary to the above theorem, we obtain the following result, essentially proved by Loewy and London in [18].

Corollary 3.28 *Let $\sigma = \{1, a+bi, a-bi\}$. Then σ is the spectrum of a nonnegative matrix if and only if inequalities* (3.17) *hold. In particular, the NIEP and the (nonsymmetric) NNIEP are equivalent for $n = 3$.*

Proof. See Remark 3.27. □

As a final note, observe that the matrix:

$$R = \begin{bmatrix} x & \dfrac{-xz}{\sqrt{x^2+y^2}} & \dfrac{-y}{\sqrt{x^2+y^2}} \\ y & \dfrac{-yz}{\sqrt{x^2+y^2}} & \dfrac{x}{\sqrt{x^2+y^2}} \\ z & \sqrt{x^2+y^2} & 0 \end{bmatrix}$$

obtained from U in the above proof by taking the real and imaginary parts of U's complex columns and re-normalizing, is a classical Soules matrix. If we let D be the following quasi-diagonal matrix:

$$D = \begin{bmatrix} 1 & 0 & 0 \\ 0 & a & b \\ 0 & -b & a \end{bmatrix}$$

we see that the matrix RDR^T is the same (up to permutation) as the matrix A constructed in (3.18). This different approach, often called the "Soules approach" to the NNIEP (which was used to successfully solve the SNIEP for $n = 3, 4$ and partially for 5 in [21]), is another means by which solutions may be constructed.

3.3.2 The NNIEP for 4×4 Matrices

We now turn to the NNIEP for $n = 4$. Note that the general NIEP for $n = 4$ has been solved in two different ways, one by Meehan [22], and another, which was obtained from the coefficients of the characteristic polynomial, by Torre-Mayo et. al. [36]. Both solutions are essentially algorithmic in nature, and to date no practical means by which the spectrum $\sigma = \{1, r, a + ib, a - ib\}$ may be characterized are available.

We begin with an analysis of the possible skew patterns in this case, which we checked with the MATLAB function `skewsp`.

Observation 3.29 *There are five equivalence classes of* 4×4 *skew patterns which allow a positive null vector and satisfy* (3.15)*. These classes have the following representatives:*

$$\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & + & - \\ 0 & - & 0 & + \\ 0 & + & - & 0 \end{bmatrix}, \quad \begin{bmatrix} 0 & 0 & + & - \\ 0 & 0 & - & + \\ - & + & 0 & 0 \\ + & - & 0 & 0 \end{bmatrix}, \quad \begin{bmatrix} 0 & 0 & + & - \\ 0 & 0 & + & - \\ - & - & 0 & + \\ + & + & - & 0 \end{bmatrix},$$

$$\begin{bmatrix} 0 & 0 & + & - \\ 0 & 0 & - & + \\ - & + & 0 & + \\ + & - & - & 0 \end{bmatrix}, \quad \begin{bmatrix} 0 & + & + & - \\ - & 0 & + & + \\ - & - & 0 & + \\ + & - & - & 0 \end{bmatrix}.$$

(Note that the third and fourth matrices in the above are signature similar via $D = \operatorname{diag}(1,-1,1,1)$.)

We are able to resolve the NNIEP for $n = 4$ for normal matrices that possess the first two skew patterns above. For ease of presentation, our constructions will utilize the following quasi-diagonal form for normal matrices:

$$\Lambda = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & r & 0 & 0 \\ 0 & 0 & a & -b \\ 0 & 0 & b & a \end{bmatrix},$$

to which our normal matrices will be real-orthogonally similar. We note also that the arrangement of the diagonal blocks in Λ is somewhat arbitrary, and additional matrices and inequalities result if we rearrange the blocks, so long as the spectral radius corresponds to the nonnegative or positive eigenvector. We intend to undertake this fully in future research.

We proceed by cases to present our current work on this problem.

Case 1. Denote by $\hat{K}$ the matrix:

$$\hat{K} = \frac{1}{\sqrt{x^2+y^2+z^2}} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & z & -y \\ 0 & -z & 0 & x \\ 0 & y & -x & 0 \end{bmatrix}.$$

We lose no generality in assuming $K = b\hat{K}$, where $\sigma(\hat{K}) = \{0, 0, i, -i\}$. Proceeding as in the proof of Theorem 3.26, an orthogonal matrix that puts $\hat{K}$ in quasi-diagonal form is:

$$S = \begin{bmatrix} w & -\sqrt{x^2+y^2+z^2} & 0 & 0 \\ x & \frac{wx}{\sqrt{x^2+y^2+z^2}} & -\frac{xz}{\sqrt{x^2+y^2}\sqrt{x^2+y^2+z^2}} & -\frac{y}{\sqrt{x^2+y^2}} \\ y & \frac{wy}{\sqrt{x^2+y^2+z^2}} & -\frac{yz}{\sqrt{x^2+y^2}\sqrt{x^2+y^2+z^2}} & \frac{x}{\sqrt{x^2+y^2}} \\ z & \frac{wz}{\sqrt{x^2+y^2+z^2}} & \frac{\sqrt{x^2+y^2}}{\sqrt{x^2+y^2+z^2}} & 0 \end{bmatrix}.$$

Observe that S is a classical Soules matrix. Now, upon examining the entries of $A = S\Lambda S^T$, we see that $A \geq 0$ if and only if the following inequalities are satisfied:

$$-\frac{w^2}{x^2+y^2+z^2} \leq r \leq 1,$$

$$-\min\left\{\frac{x^2}{y^2+z^2}, \frac{y^2}{x^2+z^2}, \frac{z^2}{x^2+y^2}\right\} \cdot (rw^2+x^2+y^2+z^2) \leq a \leq 1,$$

and

$$b \leq \min\left\{\frac{xy}{z}, \frac{xz}{y}, \frac{yz}{x}\right\} \cdot \frac{rw^2+x^2+y^2+z^2-a}{\sqrt{x^2+y^2+z^2}}.$$

As in the proof of Theorem 3.26, since $w \geq x \geq y \geq z$, we have:

$$\min\left\{\frac{x^2}{y^2+z^2}, \frac{y^2}{x^2+z^2}, \frac{z^2}{x^2+y^2}\right\} = \frac{z^2}{x^2+y^2}$$

and

$$\min\left\{\frac{xy}{z}, \frac{xz}{y}, \frac{yz}{x}\right\} = \frac{yz}{x}.$$

Thus, using $w^2+x^2+y^2+z^2=1$, it follows that $A \geq 0$ if and only if:

$$-\frac{w^2}{1-w^2} \leq r \leq 1, \tag{3.19}$$

$$-\frac{z^2(1-(1-r)w^2)}{x^2+y^2} \leq a \leq 1-(1-r)w^2, \tag{3.20}$$

$$b \leq \frac{yz(1-a-(1-r)w^2)}{x\sqrt{1-w^2}}. \tag{3.21}$$

Observe that if we let $w \to 0^+$, (3.19) becomes $0 \leq r \leq 1$, and (3.20) and (3.21) become (3.17). In this case, A is a reducible matrix.

Case 2. Let $\hat{K}$ be the following matrix:

$$\hat{K} = \frac{1}{\sqrt{w^2+x^2}\sqrt{y^2+z^2}}\begin{bmatrix} 0 & 0 & xz & -xy \\ 0 & 0 & -wz & wy \\ -xz & wz & 0 & 0 \\ xy & -yw & 0 & 0 \end{bmatrix}.$$

Proceeding as before, a matrix which puts $\hat{K}$ in quasi-diagonal form is:

$$S = \begin{bmatrix} w & \frac{w\sqrt{y^2+z^2}}{w^2+x^2} & 0 & -\frac{x^2}{\sqrt{w^2+x^2}} \\ x & \frac{x\sqrt{y^2+z^2}}{w^2+x^2} & 0 & \frac{w}{\sqrt{w^2+x^2}} \\ y & -\frac{y\sqrt{w^2+x^2}}{\sqrt{y^2+z^2}} & -\frac{z}{\sqrt{y^2+z^2}} & \\ z & -\frac{z\sqrt{w^2+x^2}}{\sqrt{y^2+z^2}} & \frac{y}{\sqrt{y^2+z^2}} & 0 \end{bmatrix}.$$

Note again that S is a classical Soules matrix. Upon examining the entries of $A = S\Lambda S^T$, we see that $A \geq 0$ if and only if the following inequalities are satisfied:

$$\begin{gathered}
-1 \leq r \leq 1, \\
a \geq -\min\left\{\frac{x^2(1-(1-r)(y^2+z^2))}{w^2}, \frac{z^2(1-(1-r)(w^2+x^2))}{y^2}\right\}, \\
a \leq \min\left\{1-(1-r)(y^2+z^2), 1-(1-r)(w^2+x^2)\right\}, \\
b \leq \min\left\{\frac{wz(1-r)}{xy}, \frac{wy(1-r)}{xz}, \frac{xz(1-r)}{wy}, \frac{xy(1-r)}{wz}\right\}.
\end{gathered}$$

Since $w \geq x \geq y \geq z > 0$, we have $w^2 + x^2 \geq y^2 + z^2$, hence:

$$1-(1-r)(y^2+z^2) \geq 1-(1-r)(w^2+x^2).$$

Also, $wy \geq wz$ and $xy \geq xz$, so

$$\frac{wy}{xz} \geq \frac{wz}{xy} \quad \text{and} \quad \frac{xy}{wz} \geq \frac{xz}{wy},$$

thus as $w^2yz \geq x^2yz$, we have:

$$\frac{wz}{xy} \geq \frac{xz}{wy}.$$

So,

$$\begin{gathered}
\min\left\{1-(1-r)(y^2+z^2), 1-(1-r)(w^2+x^2)\right\} = 1-(1-r)(w^2+x^2), \\
\min\left\{\frac{wz(1-r)}{xy}, \frac{wy(1-r)}{xz}, \frac{xz(1-r)}{wy}, \frac{xy(1-r)}{wz}\right\} = \frac{xz(1-r)}{wy}.
\end{gathered}$$

Further, if $xy \geq wz$, then

$$\frac{x^2(1-(1-r)(y^2+z^2))}{w^2} \geq \frac{z^2(1-(1-r)(w^2+x^2))}{y^2};$$

however, the ordering of the two terms in the above inequality is not certain if $wz < xy$.

Therefore, $A \geq 0$ if and only if:

$$-1 \leq r \leq 1, \tag{3.22}$$

$$-\min\left\{\frac{x^2(1-(1-r)(y^2+z^2))}{w^2}, \frac{z^2(1-(1-r)(w^2+x^2))}{y^2}\right\} \leq a \leq 1-(1-r)(y^2+z^2) \tag{3.23}$$

$$b \leq \frac{xz(1-r)}{wy} \tag{3.24}$$

The remaining cases are difficult since the orthogonal matrices we must use to put $\hat{K}$ into quasi-diagonal form contain parameters in addition to those appearing in the Perron vector. It is the subject of further research to determine the restrictions that prevail on the spectrum of the associated matrices. We suspect that the above two cases encompass the majority of possible spectra in the NNIEP for $n = 4$.

For illustration, consider the base inequalities considered in the above two cases, and momentarily ignore the ordering of w, z, y, z. In Case 1, if we let $w = 0$ and put $x = y = z = \frac{1}{\sqrt{3}}$, the inequalities become:

$$0 \leq r \leq 1,$$
$$-\frac{1}{2} \leq a \leq 1,$$
$$b \leq \frac{1-a}{\sqrt{3}},$$

which are the same as (3.17) together with $0 \leq r \leq 1$. That this is the obvious result follows from the fact that setting $w = 0$ implies then the resulting A is reducible. In

Case 2, if we take $w = x = y = z = \frac{1}{2}$, the resulting inequalities are:

$$-1 \leq r \leq 1,$$
$$-\frac{1+r}{2} \leq a \leq \frac{1+r}{2},$$
$$b \leq 1 - r.$$

If we consider solutions of the above inequalities as determining regions in $\mathbb{C}$, we see that the first set of inequalities is simply Θ_3, an equilateral triangle with vertices at $1, e^{2\pi i/3}, e^{4\pi i/3}$, while the second set is a square with vertices at $1, i, -1, -i$. Taking the union of these two sets, we obtain the following shaded set, sketched with the boundary of Θ_4 superimposed, in Figure 2.

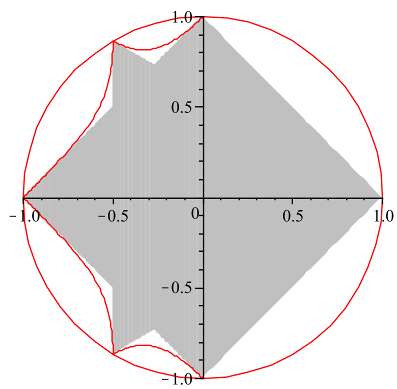


Figure 2: Known solutions to the NNIEP for $n = 4$

It is known, see [23, Chapter 7], that α is an eigenvalue of a 4×4 nonnegative circulant matrix if and only if α belongs to the set shaded in Figure 2 above. Moreover, observe that if

$$\sigma_t = \left\{1, 2t, -\frac{1}{2} - t + i\frac{1}{2}, -\frac{1}{2} - i\frac{1}{2}\right\},$$

then σ_0 is the spectrum of a nonnegative 4×4 normal matrix; it is the result of all our computations performed thus far that for no $t > 0$ is the same true of σ_t. Using Meehan's

[22] algorithm, however, we can easily construct a nonnormal nonnegative 4×4 matrix which has spectrum σ_t.

3.4 Conclusion

In this chapter, we summarized the relevant necessary and some sufficient conditions for the general NIEP, and used the latter to determine some sufficient conditions for the NNIEP. Our purpose was to make some progress on the solution of the NNIEP, which we viewed from the perspective as the problem of analyzing skew-symmetric sign patterns which allow positive null vectors, constructing the associated orthonormal sets of eigenvectors, and, in turn, using these bases to construct normal matrices.

We established necessary and sufficient conditions on a given skew pattern to possess a positive eigenvector, and qualifying these patterns up to permutation and transposition, we found that in the case $n = 3$ only one pattern, and for $n = 4$, five patterns emerged for consideration. This allowed a complete solution to the NNIEP in the case $n = 3$ (in fact, the strongest result possible), and a partial analysis of two of the five skew patterns in the case $n = 4$ was provided as well.

We believe that, through further research into the orthonormal bases for the other three skew patterns, and through a variation of the arrangement of entries in the quasi-diagonal forms used to construct realizing matrices, that a complete solution to the NNIEP in the case $n = 4$ will be possible.

Chapter 4

Concluding Remarks

In this dissertation, we investigated the implications of a property involving the spectral decomposition of symmetric matrices, and constructed some preliminary solutions to the normal nonnegative inverse eigenvalue problem (NNIEP). In Chapter 2 we studied the former problem, and we obtained a characterization of a new class of orthogonal matrices, which we call extended Soules matrices, that are generalizations of the widely-known class of Soules matrices examined in the literature (which we call classical Soules matrices). Using this characterization, we proved some results regarding matrix functions and complete positivity of matrices generated by extended Soules matrices which were only previously known to hold for classical Soules matrices. A reasonable conjecture is that any result regarding classical Soules matrices that does not have assumptions of irreducibility, or require a positive first column, also holds for extended Soules matrices. Another aspect of the afore-mentioned property is the examination of the eigenvalues involved, which was undertaken preliminarily and whose results were illustrated using certain orthogonal Hadamard matrices. This interesting application was not fully resolved, but we conjecture that a closed-form solution, i.e. one specifying the vertices of the convex hull of eigenvalues for which the resulting matrices have the spectral decomposition property, is possible.

In Chapter 3, after giving an overview of the NIEP, as well as some necessary and some sufficient conditions, we examined a new approach to the study of the NNIEP.

Namely, our approach consists the investigation of skew-symmetric matrices with positive null vectors, from which we obtain a unitary matrix that can be used to construct solution matrices. That this approach has efficacy is that its scope includes all possible skew-symmetric parts of normal matrices, and is evidenced by the solution to the NNIEP for 3×3 matrices - the strongest result possible for this case. We present also some preliminary results for the NNIEP for 4×4 matrices using this approach, which fully resolves two out of five possible cases. Interestingly, the unitary matrices constructed in these two cases, when written as orthogonal matrices, are extended Soules matrices. The remaining three cases are difficult since the unitary matrices involve parameters independent of spectral data, and so require a very careful and lengthy analysis as to the outcome of resulting inequalities. Our initial work suggests that no new lists $\sigma = \{1, r, a + ib, a - ib\}$ can be realized in these three cases that are not already realized in the first two cases - further research is required to verify this statement, however. We note also that the results obtained here are not contained in any known sufficient condition for the NNIEP adapted to 4×4 matrices. By generalizing individual skew patterns and constructing normal matrices, we believe it is possible to obtain further sufficient conditions for the NNIEP for any order that are independent of those appearing in the literature.

Appendix A

MATLAB Programs

A.1 MATLAB Code for sohad

```
function sohad(m)

format rat; % set output to belong to the set of rational numbers.


% 1.  Construct A and b.


    % a.  Construct first 2^m rows.  These rows represent the

    % inequalities for the set S_n.

        b=[-1,zeros(1,2^m-1),-ones(1,m-1)]';

        B=[eye(2^m-1);zeros(1,2^m-1)];

        C=[zeros(1,2^m-1);eye(2^m-1)];

        A=[C-B;-1,-1,zeros(1,2^m-3)]; % includes row for m=2.

        clear B;

        clear C;



    % b.  Construct last m-1 rows.  These represent the additional

    % inequalities that must be satisfied so that the resulting
```

```
    % symmetric matrix is nonnegative.

      for i=1:m-2

          c=2*[ones(1,2^i-1),zeros(1,2^m-2^i)];

          d=[ones(1,3*2^i-1),zeros(1,2^m-3*2^i)];

          A=[A;c-d];

          clear c;

          clear d;

      end



% 2.  Compute extreme points.

    % a.  Build a matrix containing rows of potential

    % extreme points, which are computed as solutions of

    % r-square subsystems of Ax=b, where r is the rank of A.

      r=rank(A);

      B=nchoosek(2:2^m+m-1,r);

      n=size(B,1);

      X=[];

      for i=1:n
```

```
        if det(A(B(i,:),:))~=0
            X(i,:)=(A(B(i,:),:)\b(B(i,:),1))';
        end
    end

    s=size(X,1);

% b.  Due to truncation error in MATLAB, small negative numbers
% are introduced that we first set equal to zero.  Then we test
% each resulting solution found in a in the original inequality
% Ax-b>=0, where again due to truncation error, we accept
% solutions which yield small negative numbers in the vector
% Ax-b.

    for i=1:s
        for j=1:r
            if abs(X(i,j))<=10^(-(m-1)*m) % set precision.
                X(i,j)=0;
            end
        end
    end



    p=1;
```

```
    for i=1:s
        for j=1:r+m
            if A(j,:)*(X(i,:)')-b(j,1)>-10^(-(m-1)*m)
            else
                p=p+1;
            end
        end
        if p>=2
            X(i,:)=zeros(1,r);
            p=1;
        end
    end
```

```
% c.  Remove any duplicate or zero rows from matrix of extreme
% points.

    unique(X,'rows')'
```

A.2 MATLAB Code for skewsp

```
function skewsp(n,s)

%  The purpose of this funcion is to search through all {0,1,-1} skew
```

```
% matrices for which each nonzero row has at least one 1 and one -1,
% and then classify the resulting patterns up to permutation and
% transposition. The function takes as input the size n of the matrix
% and a parameter s that is either 0 or 1, and provides as output the
% entries above the diagonal, and written in lexicographic order.  If
% s=0 we classify up to transposition and permutation only, and if
% s=1, we also classify up to signature similarity.


% 1.  Check that input is correct.
    if (s~=0) & (s~=1)
        disp('Error.  The second parameter must be 0 or 1.')
        return
    end


m=(n^2-n)/2; % m is the number of entries above the diagonal
A=zeros(n*m,n);
% For each consecutive set of n rows, A stores a "basic skew matrix"
% which are skew symmetric matrices with exactly one 1 above the
% diagonal and one -1 below the diagonal.


% 2.  Construct all possible n-square basic skew matrices, and stack
```

```
% one on top of the other in A.

    B=zeros(m,2);
    C=zeros(m,2);
    B(1,1)=1;
    B(m,2)=n;
    C(1,1)=2;
    C(1,2)=1;
    a=2;
    b=1;

    for i=2:m % construct indices for 1's and -1's
        if a==n-b+1
            B(i,1)=B(i-1,1)+n+1;
            B(i-1,2)=a+b-1;
            C(i,1)=B(i,1)+1;
            C(i,2)=b+1;
            b=b+1;
            a=2;
        else
            B(i,1)=B(i-1,1)+n;
            B(i-1,2)=a+b-1;
            C(i,1)=B(i,1)+a;
            C(i,2)=b;
```

```
            a=a+1;
        end
    end

    for i=1:m % place 1 & -1 indices into basic skew matrix
        A(B(i,1),B(i,2))=1;
        A(C(i,1),C(i,2))=-1;
    end

    clear B;
    clear C;

% 3.  Collect all linear combinations of basic skew matrices that have
% either no nonzero elements or at least one 1 and one -1 in each row,
% where the set of coefficients comes from the set of all combinations
% of the elements (0, 1, -1) taken m at a time.  Collect the entries
% of each appearing above the diagonal and order them lexicographically.

    D=combn([0,1,-1],m); % generate 3^m X m coefficient matrix

    for i=1:3^m % positive null vector condition
        E=D(i,1)*A(1:n,1:n);
        for j=2:m
            E=E+D(i,j)*A((j-1)*n+1:(j)*n,1:n);
```

```
        end
            F=abs(E);
            for l=1:n
                if (sum(F(l,:))~=0 & abs(sum(E(l,1:n)))==sum(F(l,:)))
                D(i,:)=zeros(1,m);
                end
            end
            clear F;
    end

    clear E;
    D(~any(D,2),:)=[]; % remove trivial linear combinations.

% 4.  Classify the result of step 3 up to transposition and permutation.

    % a.  Classify up to transposition (i.e. multiplication by -1)

        c=size(D,1);

        for i=1:c % transposition condition
            for j=i+1:c
                if (D(i,:)==-D(j,:)) D(j,:)=zeros(1,m);
                end
            end
```

```
    end

    D(~any(D,2),:)=[];
    c=size(D,1);

% b.  Construct coefficients representing permutation matrices.

    G=perms([n:-1:1]);
    f=size(G,1);
    H=zeros(n*f,n);
    g=1; % permutation counter

    for i=1:n:n*f
        for j=1:n
            H(i+j-1,G(g,j))=1;
        end
        g=g+1;
    end

    clear G;

% c.  Classify up to permutation similarity.

    for i=1:c % permutation similarity
```

```
    E=D(i,1)*A(1:n,1:n);
    for j=2:m
        E=E+D(i,j)*A((j-1)*n+1:(j)*n,1:n);
    end
    for k=i+1:c
        F=D(k,1)*A(1:n,1:n);
        for l=2:m
            F=F+D(k,l)*A((l-1)*n+1:(l)*n,1:n);
        end
        h=sum(abs(D(i,:)));
        if h~=0
            for p=n+1:n:n*f
                if (H(p:p+n-1,:)*F*(H(p:p+n-1,:))'==E)
                    D(k,:)=zeros(1,m);
                end
            end
        end
    end
end

D(~any(D,2),:)=[];

d=size(D,1);
```

```
% 5.  (Optional)  Classify up to signature similarity.

    if s==1

        % a.  Generate all possible signature matrices, and collect only
        % diagonal entries.

            J=combn([1,-1],n);
            e=size(J,1);

        % b.  Remove skew coefficients that are signature similar.

            for i=1:d % signature similarity
                E=D(i,1)*A(1:n,1:n);
                for j=2:m
                    E=E+D(i,j)*A((j-1)*n+1:(j)*n,1:n);
                end
                for l=i+1:d
                    F=D(l,1)*A(1:n,1:n);
                    for p=2:m
                        F=F+D(l,p)*A((p-1)*n+1:(p)*n,1:n);
                    end
                    for q=2:e
                        if (diag(J(q,1:n))*F*diag(J(q,1:n))==E)
```

```
                        D(1,:)=zeros(1,m);
                    end
                end
            end


        end
        D(~any(D,2),:)=[];
        D
else
    D
end
```

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