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On certain sets of matrices: Euclidean squared distance matrices, ray-nonsingular matrices and matrices generated by reflections

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ON CERTAIN SETS OF MATRICES

Euclidean squared distance matrices,

ray-nonsingular matrices and

matrices generated by reflections

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I would like to dedicate this dissertation to my wife, Amy. Without your love and support, I would never reach my dreams. And to my children, David, Alexandra, Megan and Nathaniel. Sometimes it was only by watching you grow and learn that I remember that learning is fun and to ENJOY my "work".

Contents

Acknowledgements **vi**

List of Figures **vii**

List of Tables **viii**

Abstract **ix**

1 Introduction **2**

1.1 Notation and Definition 2

1.2 Overview 4

2 Euclidean Squared Distance Matrices **7**

2.1 Characterization of ESD Matrices 8

2.2 Consequences of the Characterizations of $\mathcal{D}(n)$ 27

2.3 Uniqueness of Completions 42

2.4 Spherical ESD Matrices 58

3 Ray-Nonsingular Matrices **74**

3.1 Introduction 74

3.2 Preliminary Results and Strategies of Proof 75

3.3 Sufficient Conditions for 3×3 Patterns to be Strongly Balanceable . 78

3.4 Proof of Main Theorem 83

3.5 Figures and Tables 115

4 Finite Reflection Groups **121**

4.1 Introduction and Background 121

4.2 Preliminary Results 124

4.3 $\mathbf{H}_3$ 126

4.4 $\mathbf{H}_4$ 131

4.5 $\mathbf{F}_4$ 139

4.6 $\mathbf{E}_8$ 145

4.7 $\mathbf{E}_7$ 152

4.8 $\mathbf{E}_6$ 160

4.9 MATLAB Programs 168

Bibliography **178**

Vita **185**

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List of Figures

3.1 Graphical Representation of $R(0,0)$ 79

3.2 Graphical Representation of $R(\alpha,\beta)$ 79

3.3 Representations of $R(0,0) \cap R(\alpha,\beta)$ for Forms (1) - (4) 115

3.4 Representations of $R(0,0) \cap R(\alpha,\beta)$ for Forms (5) - (10) 116

3.5 Representations of $R(0,0) \cap R(\alpha,\beta)$ for Forms (11) - (C4) 117

3.6 Representations of $R(0,0) \cap R(\alpha,\beta)$ for Forms (C5) - (C12) 118

List of Tables

3.1 Classes of vectors 81

3.2 Intersection of solution sets. 119

3.3 Conditions for empty intersection of the two solution sets. 120

Abstract

In this dissertation, we study three different sets of matrices. First, we consider Euclidean distance squared matrices. Given n points in Euclidean space, we construct an $n \times n$ Euclidean squared distance matrix by assigning to each entry the square of the pairwise interpoint Euclidean distance. The study of distance matrices is useful in computational chemistry and structural molecular biology. The purpose of the first part of the thesis is to better understand this set of matrices and its different characterizations so that a number of open problems might be answered and known results improved. We look at geometrical properties of this set, investigate forms of linear maps that preserve this set, consider the uniqueness of completions to this set and look at subsets that form regular figures. In the second part of this thesis, we consider ray-pattern matrices. A ray-pattern matrix is a complex matrix with each nonzero entry having modulus one. A ray-pattern is said to be ray-nonsingular if all positive entry-wise scalings are nonsingular. A full ray-pattern matrix has no zero entries. It is known that for $n > 5$, there are no full ray-nonsingular matrices but examples exist for $n < 5$. We show that there are no 5×5 full ray-nonsingular matrices. The last part of this thesis studies certain of the finite reflection groups. A reflection is a linear endomorphism T on the Euclidean space V such that $T(v) = v - 2(v, u)u$ for all $v \in V$. A reflection group is a group of invertible operators in the algebra of linear endomorphism on V that are generated by a set of reflections. One question that has recently been studied is the form of linear operators that preserve finite reflection groups. We first discuss known results about preservers of some finite reflection groups. We end by showing the forms of the remaining open cases.

ON CERTAIN SETS OF MATRICES

Euclidean squared distance matrices, Ray-nonsingular matrices

and matrices generated by reflections

Chapter 1

Introduction

The theme of this dissertation is the study of certain sets of matrices. We will consider different open problems for each of these sets. To begin, we will first give some basic definitions and notation. Then we will give an overview of the remaining chapters.

1.1 Notation and Definition

We use $\mathbf{R}$ and $\mathbf{C}$ to denote the real and complex fields. The set of $m \times n$ matrices with entries from a field $\mathbf{F}$ are denoted by $M_{m,n}(\mathbf{F})$. For convenience, when $\mathbf{F} = \mathbf{R}$, we will shorten this to $M_{m,n}$. Also, we will use $M_n(\mathbf{F})$ to denote $M_{n,n}(\mathbf{F})$. For $x \in \mathbf{C}$, let $\overline{x}$ denote the complex conjugate of x and $|x|$ denote the absolute value of x. We use $\|\cdot\|$ to denote the usual Euclidean norm. For a matrix $A \in M_{m,n}(\mathbf{F})$, we use $A = (a_{ij})$ to denote that $a_{ij} \in \mathbf{F}$ is the entry of A lying in the ith row and jth column. Let $A \in M_{m,n}(\mathbf{F})$, then the $n \times m$ matrix A^t is the transpose of A, while $|A| = (|a_{ij}|)$

is the matrix of absolute values of entries of A, $\overline{A} = (\overline{a_{ij}})$ is the matrix of complex conjugates of entries of A and $A^* = \overline{A}^t$ is the Hermitian adjoint of A. Given matrices $A, B \in M_{m,n}$, $A \circ B$ is also in $M_{m,n}$ and is the entrywise product of A and B. It is called the Hadamard (or Schur) product.

Let $I \in M_n(\mathbf{F})$ be the identity matrix. Let $e_1, \ldots, e_n$ be the vectors forming the standard basis for $\mathbf{R}$. In other words, e_i is the vector with the only nonzero entry in the ith position and the value of that entry equal to one. Let e be the vector of all ones. Let E_{ij} be a standard basis matrix of $M_{m,n}$. In other words, E_{ij} is the matrix whose only nonzero entry is in the ith row and jth column and is equal to one. For M_n, $E_{ij} = e_i e_j^t$. Let J be the all ones matrix. For $A \in M_{p,q}$ and $B \in M_{r,s}$, the matrix $A \oplus B \in M_{p+r,q+s}$ is the direct sum and defined as

$$A \oplus B = \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix}.$$

For any vector $v \in \mathbf{F}^n$, then $D = \text{diag}(v) \in M_n(\mathbf{F})$ is the diagonal matrix with $(D)_{ii} = v_i$.

A matrix $A \in M_n(\mathbf{F})$ is symmetric if $A^t = A$. A is Hermitian if $A^* = A$. Note that for $M_n(\mathbf{R})$, the properties of being Hermitian and symmetric are the same. Let S_n be the set of real $n \times n$ symmetric matrices. A matrix $A \in M_n(\mathbf{F})$ is said to be positive (semi-)definite if $x^*Ax > 0$ (respectively, $x^*Ax \geq 0$) for all $0 \neq x \in \mathbf{F}^n$. Alternatively, A is Hermitian and all the eigenvalues of A are positive (respectively, nonnegative). Let $\text{PD}(n)$ be the set of real $n \times n$ positive definite matrices and $\text{PSD}(n)$ the set of real $n \times n$ positive semi-definite matrices. It is an easily proven fact that a matrix $A = (a_{ij}) \in \text{PSD}(n)$ if and only there exists a matrix $X \in M_{k,n}(\mathbf{F})$ such that $A = X^*X$. Furthermore, the rank of A and X agree. If we label the columns of X as $x_1, \ldots, x_n \in \mathbf{F}^k$, then $a_{ij} = (x_i, x_j)$ where $(\cdot, \cdot)$ is the standard inner product. Such matrices are called Gram matrices.

1.2 Overview

This thesis deals with three different sets of matrices:

In Chapter 2 we study the cone of Euclidean squared distance (ESD) matrices. Given n points in Euclidean space, we can construct an $n \times n$ Euclidean distance matrix by assigning to each entry of the matrix the pairwise interpoint Euclidean distance. The study of distance matrices was motivated originally by statisticians and psychometricians interested in (classical) multidimensional scaling and by more recent work which involves computational chemistry and structural molecular biology. The purpose of this chapter is to better understand this set and its different characterizations so that a number of open problems might be answered and known results improved. We start the chapter describing the motivation for studying this set of matrices and then review different characterizations of this set and their history. We then present some results on the facial structure of the convex cone, the angle between matrices in the set and linear preservers of this set. The third section will deal with the uniqueness of a completion to this set of ESD matrices. In a partial matrix, some entries are given and others are left unknown. A completion of the partial matrix is a matrix whose entries agree in the specified locations of the partial matrix and the unspecified entries have values assigned so that the matrix takes on the desired properties. We consider the problem of testing the uniqueness of a given completion. We generalize this result so that other completion problems might also be considered. In the last section, we consider a subset of Euclidean squared distance matrices, namely those that correspond to points that lie on a hypersphere whose center is the origin and the centroid of the points is also the origin. We discuss known results, especially characterizations, and then consider the form of linear preserver of this set.

In Chapter 3, we consider ray-pattern matrices. This is a generalization of sign-pattern matrices. A ray-pattern is a complex matrix with each nonzero entry having modulus one. A ray-pattern A is said to be ray-nonsingular if $A \circ X$ is nonsingular for each entry-wise positive matrix X. Looking at full ray-pattern matrices, i.e. no zero entries, it is known that for $n > 5$, there are no $n \times n$ full ray-nonsingular matrices. For $n < 5$ there are examples of full ray-nonsingular matrices. We show that for $n = 5$ there are no full ray-nonsingular matrices.

The last chapter of this thesis studies various sets of matrices generated by reflections. Recall that a reflection is a linear endomorphism T on the Euclidean space V such that $T(v) = v - 2(v, u)u$ for all $v \in V$. A reflection group is a group of invertible operators in the algebra of linear endomorphism on V that are generated by a set of reflections. These reflections can be represented by matrices and the resulting reflection groups are matrix sets. The particular problem that we study involves linear preservers of the space spanned by these reflection groups. We study this problem by considering the representative matrix sets $\mathcal{S}$ and then determine the form of those linear operators $\psi : [\mathcal{S}] \mapsto [\mathcal{S}]$ such that $\psi(\mathcal{S}) = \mathcal{S}$. We first discuss known results about preservers of some finite reflection groups and then solve the problem for the remaining open cases.

Sections 2.1 and 2.2 are based on joint work with Chi-Kwong Li and Michael Trosset and found in [34]. Section 2.3 is based on [32], which is joint work with my advisor, Chi-Kwong Li. Chapter 3 represents joint work with Chi-Kwong Li and Bryan Shader and is based on [33]. Chapter 4 is based on [31], joint work with Chi-Kwong Li.

Chapter 2

Euclidean Squared Distance Matrices

We divide this chapter into four sections. In the first section, we will give background information about the set of Euclidean squared distance (ESD) matrices. This will include motivation for studying this problem, different characterizations of this set, as well as a short history of the study of this problem. The second section will deal with some consequences of these characterizations. We will present results concerning the facial structure of the cone of $n \times n$ Euclidean squared distance matrices, bounds on angles between certain matrices and a discussion on linear preservers of this set. The third section will study the uniqueness of a completion of a partial matrix to an ESD matrix. The final section will address future work. In particular, we will discuss a subset of $\mathcal{D}(n)$ whose elements we call spherical ESD matrices.

One of the interesting facets of the study of ESD matrices is that the characterizations mentioned in this next section provide a relationship between the set of ESD matrices and other types of matrices. To study $n \times n$ ESD matrices, originally $(n+1) \times (n+1)$ Menger matrices were studied. More recently, a subset of $n \times n$ positive semidefinite (PSD) matrices have been extensively studied. Our results use extensively $(n-1) \times (n-1)$ PSD matrices. Throughout this chapter, we will use these other sets of matrices to study the set of ESD matrices. Not only does this allow us to more easily say something about ESD matrices, but in some cases (see subsection 2.3.3) to say something about other problems too.

2.1 Characterization of ESD Matrices

2.1.1 Motivation

Distance geometry is concerned with the interpoint distances of configurations of n points in metric spaces. It is natural to organize these interpoint distances in the form of an $n \times n$ *distance matrix*, so the study of distance geometry inevitably borrows tools from matrix theory. For example, a fundamental problem in distance geometry is the embedding problem: determine whether or not a specified set of numbers can be realized as a configuration of points in a specified metric space. This problem was first addressed (anonymously) in 1841 by A. Cayley [9], who derived a necessary condition involving a matrix determinant for five points to reside in Euclidean space.

The ability to characterize distance matrices has important applications in a variety of disciplines. Nearly a century after Cayley's contribution, a characterization of distance matrices (re)discovered by G. Young and A.S. Householder [50] was the impetus for (classical) multidimensional scaling [43, 46, 17]. Originally developed by psychometricians and statisticians, multidimensional scaling is a widely used tool for data visualization and dimension reduction. Research on multidimensional scaling continues to exploit facts about distance matrices, e.g., [38]. Analogously, in computational chemistry and structural molecular biology, the problem of determining a molecule's 3-dimensional structure from information about its interatomic distances is the problem of finding a matrix of 3-dimensional Euclidean distances that satisfies certain constraints, as in [11].

Characterizations of distance matrices are not only mathematically elegant, but genuinely useful to researchers in other disciplines. Unfortunately, the literature is fragmented and somewhat obscure. We have endeavored to collect several well-known characterizations of Euclidean squared distance matrices. Applying the tools of modern matrix theory, we provide short proofs of these characterizations and derive several consequences of them.

Formally, a *Euclidean squared distance (ESD)* matrix $A = (a_{ij})$ is a matrix for which there exist $x_1, \ldots, x_n \in \mathbf{R}^k$ such that $a_{ij} = \|x_i - x_j\|^2$. If k is the smallest dimension for which such a construction is possible, then k is the *embedding dimension* of A. Clearly, the choice of $x_1, \ldots, x_n$ is not unique, for if $\tilde{x}_i = x_i - x_0$ then $\tilde{x}_i - \tilde{x}_j = x_i - x_j$. Given $w \in \mathbf{R}^n$ with $\sum_{j=1}^n w_j = e^t w \neq 0$, let $x_0 = \sum_{j=1}^n w_j x_j / \sum_{j=1}^n w_j$. Then $\sum_{j=1}^n w_j \tilde{x}_j = 0 \in \mathbf{R}^k$, so we can assume without loss of generality that $\sum_{j=1}^n w_j x_j = 0 \in \mathbf{R}^k$. This linear dependence of the vectors $x_1, \ldots, x_n$ demonstrates the well-known fact that the largest possible embedding dimension for n points is $n-1$.

It follows immediately from the definition that an ESD matrix is a real, symmetric, nonnegative, hollow ($a_{ii}=0$) matrix. These properties are necessary but not sufficient for a matrix to be an ESD matrix (a matrix with these properties is called a *pre-distance* or *dissimilarity* matrix); in Subsection 2.1.2 we collect and provide short proofs (some new) of a number of well-known characterizations of ESD matrices.

Let $\mathcal{D}(n)$ denote the set of $n\times n$ ESD matrices. Suppose that $A=(\|x_i-x_j\|^2)\in\mathcal{D}(n)$ and $\alpha\geq 0$. Then $(\|\alpha x_i-\alpha x_j\|^2)=\alpha^2 A\in\mathcal{D}(n)$, and note that therefore $\mathcal{D}(n)$ is a cone. In the next section we will show that it is a convex cone.

2.1.2 Characterizations

Let $\mathbf{S}_n$ be the set of $n\times n$ symmetric matrices. Let $e_1,\ldots,e_n$ denote the coordinate unit vectors in $\mathbf{R}^n$ and let I denote the $n\times n$ identity matrix. Set $e=e_1+\cdots+e_n$ and $J=ee^t$. Given $w\in\mathbf{R}^n$ such that $e^tw\neq 0$, define the linear mapping $\tau_w:\mathbf{S}_n\to\mathbf{S}_n$ by

$$\tau_w(A)=-\frac{1}{2}\left(I-\frac{ew^t}{e^tw}\right)A\left(I-\frac{we^t}{e^tw}\right). \tag{2.1.1}$$

Given $w\in\mathbf{R}^n$, we say that $x_1,\ldots,x_n\in\mathbf{R}^k$ is *w-centered* if and only if $\sum_{j=1}^n w_jx_j=0$. The following theorem offers characterizations of the ESD matrices. The historical context of these characterizations are discussed in the next section.

Theorem 2.1 *Suppose that A is an $n\times n$ pre-distance matrix. Let w be any vector in $\mathbf{R}^n$ such that $e^tw\neq 0$ and let U be any $n\times(n-1)$ matrix for which the $n\times n$ matrix $V=(\frac{e}{\sqrt{n}}|U]$ is orthogonal. Then the following conditions are equivalent.*

(a) *There exists a* w*-centered spanning set of* $\mathbf{R}^k$, $\{x_1, \ldots, x_n\}$, *for which* $A = (\|x_i - x_j\|^2)$.

(b) *There exists a* w*-centered spanning set of* $\mathbf{R}^k$, $\{x_1, \ldots, x_n\}$, *for which* $\tau_w(A) = (x_i^t x_j)$.

(c) *The matrix* $U^t AU$ *is negative semidefinite of rank* k.

(d) *The submatrix* B *in*

$$\hat{A}_0 = \begin{pmatrix} 1 & 0 \\ 0 & V^t \end{pmatrix} \begin{pmatrix} 0 & e^t \\ e & A \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & V \end{pmatrix} = \begin{pmatrix} 0 & \sqrt{n} & 0 \\ \sqrt{n} & * & * \\ 0 & * & B \end{pmatrix}$$

is negative semidefinite of rank k.

(e) *The matrix* $A_0 = \begin{pmatrix} 0 & e^t \\ e & A \end{pmatrix}$ *has nonzero eigenvalues* $a_1 > 0 > a_2 \geq \cdots \geq a_{k+2}$.

(f) *There exists an* $n \times n$ *permutation matrix* P *for which the matrix* $\begin{pmatrix} 0 & e^t \\ e & P^t AP \end{pmatrix}$ *has rank* $k+2$, *and, for* $j = 2, \ldots, k+2$, *each* $j \times j$ *leading principal minor is nonzero and has sign* $(-1)^{j-1}$.

Proof We first establish the equivalence of conditions (a), (b), and (c).

(c) $\Rightarrow$ **(b)** Let $v_1, \ldots, v_n$ denote the rows of V and let $u_1, \ldots, u_n$ denote the rows of U. It follows from

$$I = VV^t = \left(\tfrac{e}{\sqrt{n}} \quad U \right) \begin{pmatrix} e^t/\sqrt{n} \\ U^t \end{pmatrix} = \frac{1}{n} J + UU^t$$

that $UU^t = I - \frac{1}{n}J$. Hence, it follows from $J\frac{we^t}{e^tw} = \frac{ee^twe^t}{e^tw} = ee^t = J$ that

$$UU^t\left(I - \frac{we^t}{e^tw}\right) = \left(I - \frac{1}{n}J\right)\left(I - \frac{we^t}{e^tw}\right) = \left(I - \frac{we^t}{e^tw}\right) - \frac{1}{n}(J - J) = \left(I - \frac{we^t}{e^tw}\right).$$

Because U^tAU is a negative semidefinite matrix and has rank k, we can write $-\frac{1}{2}U^tAU = Y^tY$ for some $k \times (n-1)$ matrix Y of rank k. Let $W = U^t(I - \frac{we^t}{e^tw})$ and let $x_1, \ldots, x_n$ denote the columns of $X = YW$. Then

$$\sum_{j=1}^{n} w_j x_j = Xw = YU^t\left(I - \frac{we^t}{e^tw}\right)w = YU^t(w - w) = 0$$

and

$$\begin{aligned} X^tX &= W^tY^tYW = -\frac{1}{2}W^tU^tAUW = -\frac{1}{2}\left(I - \frac{we^t}{e^tw}\right)^t UU^tAUU^t\left(I - \frac{we^t}{e^tw}\right) \\ &= -\frac{1}{2}\left(I - \frac{ew^t}{e^tw}\right)A\left(I - \frac{we^t}{e^tw}\right) = \tau_w(A). \end{aligned}$$

It remains to show that $x_1, \ldots, x_n$ spans $\mathbf{R}^k$. The range space of U is $e^\perp$. If $z \in e^\perp$, then

$$\left(I - \frac{we^t}{e^tw}\right)z = z; \tag{2.1.2}$$

hence, U^t and $U^t(I - \frac{we^t}{e^tw})$ have the same range space. Furthermore, because $YU^t = (0|Y)V^t$, rank $YU^t =$ rank $Y = k$. Hence,

$$\text{rank } X = \text{rank } YW = \text{rank } YU^t\left(I - \frac{we^t}{e^tw}\right) = \text{rank } YU^t = k.$$

(b) $\Rightarrow$ (a) Define $\kappa : \mathrm{S}_n \to \mathrm{S}_n$ by

$$\kappa(B) = \mathrm{diag}(B)J - 2B + J\mathrm{diag}(B). \tag{2.1.3}$$

Let $X = (x_1|\cdots|x_n)$ and

$$H = \kappa\left(X^tX\right) = \left(x_i^tx_i - 2x_i^tx_j + x_j^tx_j\right) = \left(\|x_i - x_j\|^2\right). \tag{2.1.4}$$

Because $J(I - \frac{we^t}{e^t w}) = J - J = 0$ and $X(I - \frac{we^t}{e^t w}) = X - \frac{Xwe^t}{e^t w} = X$,

$$\tau_w(H) = -\frac{1}{2}\left(I - \frac{ew^t}{e^t w}\right)\left(DJ - 2X^tX + JD\right)\left(I - \frac{we^t}{e^t w}\right) = X^tX = \tau_w(A)$$

where $D = \text{diag}(B)$. Furthermore, it follows from (2.1.2) that

$$\left(I - \frac{we^t}{e^t w}\right)(e_i - e_j) = e_i - e_j,$$

so

$$\begin{aligned} H_{ij} &= -\frac{1}{2}(e_i - e_j)^t H (e_i - e_j) = (e_i - e_j)^t \tau_w(H)(e_i - e_j) \\ &= (e_i - e_j)^t \tau_w(A)(e_i - e_j) = A_{ij}, \end{aligned}$$

i.e., $H = A$.

Notice that this argument demonstrates that τ_w is injective on the hollow symmetric matrices.

(a) $\Rightarrow$ (c) Let $x_0 = \sum_{j=1}^n x_j/n$ and $\tilde{x}_i = x_i - x_0$, so that $\tilde{x}_1, \ldots, \tilde{x}_n$ is an e-centered spanning set of $\mathbf{R}^k$ with $A = (\|\tilde{x}_i - \tilde{x}_j\|^2)$. Let $\tilde{X}$ denote the $k \times n$ matrix with columns $\tilde{x}_1, \ldots, \tilde{x}_n$. Then $\tilde{X}e = 0$, so $\tilde{X}V = (0|\tilde{X}U)$ and it follows that rank $\tilde{X}U$ = rank $\tilde{X} = k$.

Because V is orthogonal, $U^te = 0$ and therefore $U^tJ = U^tee^t = 0 = JU$. Applying (2.1.4),

$$U^tAU = U^t\left(JD - 2\tilde{X}^t\tilde{X} + DJ\right)U = -2U^t\tilde{X}^t\tilde{X}U = -2\left(\tilde{X}U\right)^t\left(\tilde{X}U\right)$$

is a negative semidefinite matrix of rank k.

(c) ⇔ (d) Because $U^t e = 0$,

$$\hat{A}_0 = \begin{pmatrix} 1 & 0 \\ 0 & V^t \end{pmatrix} \begin{pmatrix} 0 & e^t \\ e & A \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & V \end{pmatrix} = V_0^t A_0 V_0 \tag{2.1.5}$$

$$= \begin{pmatrix} 1 & 0 \\ 0 & e^t/\sqrt{n} \\ 0 & U^t \end{pmatrix} \begin{pmatrix} 0 & e^t \\ e & A \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & e/\sqrt{n} & U \end{pmatrix} = \begin{pmatrix} 0 & \sqrt{n} & 0 \\ \sqrt{n} & e^t A e/n & * \\ 0 & * & U^t A U \end{pmatrix} \tag{2.1.6}$$

Thus, $B = U^t A U$ and conditions (c) and (d) are equivalent.

Now we establish the equivalence of conditions (d), (e), and (f). To do so, we rely on the following interlacing inequalities (see, for example, [14]):

If $b_1 \geq \cdots \geq b_r$ are the eigenvalues of an $r \times r$ principal submatrix of an $s \times s$ symmetric matrix with eigenvalues $a_1 \geq \cdots \geq a_s$, then $a_i \geq b_i \geq a_{s-r+i}$ for $i = 1, \ldots, r$.

(d) ⇒ (e) Because V is orthogonal, so is V_0 and it follows from (2.1.5) that A_0 and $\hat{A}_0$ have the same eigenvalues. By interchanging the first two rows of $\hat{A}_0$ and performing Gaussian elimination, we see that rank A_0 = rank $\hat{A}_0 = 2+$rank $B = 2+k$. Because $\begin{pmatrix} 0 & 0 \\ 0 & B \end{pmatrix}$ has no positive eigenvalues and is a principal submatrix of $\hat{A}_0$, it follows from the interlacing inequalities that $\hat{A}_0$, hence A_0, has at most one positive eigenvalue. But the leading 2×2 principal submatrix of A_0 has a negative determinant and therefore one positive and one negative eigenvalue; hence, by the interlacing inequalities, A_0 has at least one positive eigenvalue. Thus, A_0 has exactly one positive eigenvalue and, because rank $A_0 = k + 2$, $k + 1$ negative eigenvalues.

(e) ⇒ (d) We have already argued that rank B = rank $\hat{A}_0 - 2$ = rank $A_0 - 2 = k + 2 - 2 = k$. Given $v \in \mathbf{R}^{n-1}$, we demonstrate that $b = v^t B v \leq 0$. Toward that end, let

$$D = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & v^t \end{pmatrix} \hat{A}_0 \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & v \end{pmatrix} = \begin{pmatrix} 0 & \sqrt{n} & 0 \\ \sqrt{n} & c & * \\ 0 & * & b \end{pmatrix},$$

where $c = e^t Ae/n$. Notice that $\det(D) = -nb$.

Let $d_1 \geq d_2 \geq d_3$ denote the eigenvalues of D. Let Q be any orthogonal matrix of the form

$$Q = \left(\begin{array}{ccc|c} 0 & 1 & 0 & \\ 1 & 0 & 0 & * \\ 0 & 0 & v & \end{array}\right),$$

in which case $Q^t \hat{A}_0 Q = \begin{pmatrix} D & * \\ * & * \end{pmatrix}$ has the same eigenvalues as $\hat{A}_0$, i.e., the same eigenvalues as A_0. Because D is a principal submatrix of $Q^t \hat{A}_0 Q$, it follows from the interlacing inequalities that $d_3 \leq d_2 \leq 0$. Furthermore, it follows from the Rayleigh-Ritz Theorem that $d_1 \geq 0$. We conclude that $b = -\det(D)/n = -d_1 d_2 d_3/n \leq 0$.

(e) ⇒ (f) Any matrix of the form

$$\begin{pmatrix} 0 & e^t \\ e & P^t AP \end{pmatrix}, \tag{2.1.7}$$

where P is an $n \times n$ permutation matrix, must have the same eigenvalues as A_0. It follows from (e) that any such matrix must have rank $k + 2$. We choose P so that, for $j = 2, \ldots, k + 2$, the $j \times j$ leading principal submatrices of (2.1.7) have no zero eigenvalues. Then the 2×2 leading principal submatrix is $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, which has a positive eigenvalue. Hence, for $j = 2, \ldots, k+2$, each $j \times j$ leading principal submatrix will have one positive and $j-1$ negative eigenvalues and the corresponding minors will have signs $(-1)^{j-1}$.

(f) ⇒ (e) Because (2.1.7) has rank $k+2$, so does A_0. Because the 2×2 leading principal minor of (2.1.7) is negative, the 2×2 leading principal submatrix has one positive and one negative eigenvalue. Because the 3×3 leading principal minor of (2.1.7) is positive, it follows from the interlacing inequalities that the 3×3 leading principal submatrix has one positive and two negative eigenvalues. Continuing in this manner, we conclude that the $(k+2) \times (k+2)$ leading principal submatrix, hence (2.1.7), hence A_0, has one positive and $k+1$ negative eigenvalues. □

2.1.3 Historical background and related results

Let us make some remarks about the characterizations established in Theorem 2.1. We have already noted that the requirement that $x_1, \ldots, x_n$ is w-centered entails no loss of generality; hence, condition (a) is simply the definition of a k-dimensional ESD matrix, i.e., an ESD matrix with embedding dimension k.

A connection between the ESD matrix A and the bordered matrix A_0, from condition (e), was originally established by Cayley [9]. Bordering A on the bottom and right, Cayley demonstrated that $\det \begin{pmatrix} A & e \\ e^t & 0 \end{pmatrix} = 0$ if $A \in \mathcal{D}(n)$ for $n = 3, 4, 5$ and certain embedding dimensions. Menger [40, 41] elaborated on this connection.[1] Given A, let $A(i)$ denote the $(n-1)\times(n-1)$ submatrix of A obtained by deleting row i and column i. Obviously, if $A \in \mathcal{D}(n)$, then each $A(i) \in \mathcal{D}(n-1)$. Suppose, conversely, that each $A(i) \in \mathcal{D}(n-1)$. Then Menger's Third Fundamental Theorem [41, p. 738] states that $A \in \mathcal{D}(n)$ if and only if the sign of $\det(A_0)$ equals $(-1)^n$ or 0. This led Menger to a recursive Metrical Characterization of Euclidean Sets [41, p. 744], the first characterization of ESD matrices. Menger's hypotheses were subsequently weakened by Blumenthal [6].[2] Our condition (f) is Theorem 42.3 in [7, p. 104].

It is not easy to determine whether or not A is an ESD matrix by checking condition (f).[3] Furthermore, condition (f) is not constructive, i.e., it does not produce a configuration of points for which $A = (\|x_i - x_j\|^2)$ if A is an ESD matrix. In 1935, a constructive alternative to the Cayley-Menger approach was noted by Schoenberg [44]. Upon renumbering Schoenberg's vertices $1, \ldots, n$ as $x_1, \ldots, x_{n-1}$ and relabelling

[1]The matrices A_0 are often called Cayley-Menger matrices; their determinants are often called Cayley-Menger determinants.

[2]K. Menger and L.M. Blumenthal were the two most significant figures in classical distance ("metrical") geometry. In [41, p. 721], Menger expressed his "thanks to Dr. Leonard M. Blumenthal for his help in the editing of this paper..." In the preface to his University of Missouri monograph [5, p. 3], Blumenthal attributed his "interest in abstract metrics" to "lectures that Karl Menger gave at the Rice Institute the spring of 1931" and to "the second year [1934–35] of [a National Research Fellowship] spent with Professor Menger at the University of Vienna."

[3]Computational applications of Cayley-Menger determinants include [28], in which Klapper and DeBrota inferred a matrix of interatomic distances from bond lengths, geminal distances, and vicinal distances; and [11], in which Crippen and Havel used a "tetrangle inequality" to smooth lower and upper bounds on interatomic distances.

his vertex 0 as x_n, his Theorem 1 states that, with $w = e_n$, $\tau_w(A)$ is positive semidefinite and of rank k. In contrast to our statement of condition (b), Schoenberg did not emphasize the Gram matrix representation $\tau_w(A) = (x_i^t x_j)$; however, his proof of sufficiency is constructive and he did emphasize that "the actual construction... is therefore carried out by a reduction of the quadratic form... to its canonical form..." Three years later, condition (b) with $w = e_n$ was rediscovered by Young and Householder [50].[4] In contrast to [44], their proof used "a matrix first given by Cayley in 1841," the rank of which they demonstrated to equal $k + 2$; however, it appears that Young and Householder were unaware of earlier work by Menger and Schoenberg.[5]

If $x_1, \ldots, x_n$ is e_n-centered, then x_n is located at the origin. In contrast to [50, 43], Torgerson [46] preferred locating the configuration's centroid at the origin. Accordingly, Torgerson popularized the use of $w = e$ in condition (b). A thorough analysis

[4] G. Young received his M.S. from the University of Chicago (U.C.) in 1936 and remained as a research assistant in mathematical biophysics through 1940. A.S. Householder received his Ph.D. from U.C. in 1937. They were motivated by the interest of various U.C. psychologists in scaling, noting: "This paper was written in response to suggestions by Harold Gulliksen and by M.W. Richardson. The latter is working on a psychophysical problem in which the dimensionality of a set of points whose mutual distances are available is a central idea." Accordingly, [50] was published in *Psychometrika* and was widely cited by psychometricians unfamiliar with [44]. Richardson's paper, [43], was the seminal work on multidimensional scaling. In 1946, Gulliksen [20] surveyed methods for scaling via the method of paired comparisons; he subsequently directed the Ph.D. thesis of W.S. Torgerson, who extended Richardson's ideas to the case of fallible data in [46].

[5] In his monumental treatise on distance geometry [7], Blumenthal correctly attributed condition (b) with $w = e_n$ to [44]. He did not cite [50].

of the linear transformation τ_e was undertaken by Critchley [12], who introduced the now-ubiquitous τ to honor Torgerson. The extension of condition (b) to arbitrary $w \notin e^\perp$ is due to Gower [18, 19]. This condition is considered by many to be the most practical; not only does it give a method of verifying if a matrix is an ESD matrix, but also a straigtforward decomposition gives a realization of the generating points $x_1, \ldots, x_n \in \mathbf{R}^k$.

Both Schoenberg [44] and Young and Householder [50] gave (different) direct proofs that conditions (a) and (b) are equivalent. In contrast, Blumenthal [7] first proved that (a) and (f) are equivalent, then demonstrated that (f) and (b) are equivalent. Having thus demonstrated the equivalence of (a) and (b), he then argued that (b) and (c) are equivalent and stated the equivalence of (a) and (c) as a corollary. Although Blumenthal did not emphasize this result, we regard (c) as the fundamental characterization of ESD matrices. Condition (c) states simply that the compression of A on $e^\perp$, i.e., the restriction of both the domain and the range of the operator A to the subspace $e^\perp$, is negative semidefinite. As it does not depend on the choice of w and U, it is as nearly a coordinate-free characterization of $\mathcal{D}(n)$ as can be managed.

Because of (c), any coordinatization of $e^\perp$ leads to a characterization of ESD matrices. We note two examples from the literature.

Corollary 2.2 (Hayden and Wells [21]) *Suppose that A is an $n \times n$ pre-distance matrix. Let Q denote a Householder transformation that satisfies $Qe = -\sqrt{n}e_1$, let q denote the first column of Q, and write $Q = (q|-U)$. Then $A \in \mathcal{D}(n)$ with embedding dimension k if and only if $(-U)^t A(-U) = U^t AU$ is negative semidefinite of rank k.*

Proof Let $r_1^t, \ldots, r_n^t$ denote the rows of Q. Because $Qe = -\sqrt{n}e_1$, $r_2, \ldots, r_n \in e^\perp$. Because Householder transformations are symmetric and orthogonal, we deduce that $q = r_1 = -e/\sqrt{n}$, then apply (c) to $V = -Q$. □

Corollary 2.3 (Hayden, Wells, Liu, Tarazaga [23]) *Suppose that A is an $n \times n$ pre-distance matrix. Then $A \in \mathcal{D}(n)$ with embedding dimension k if and only if there exist mutually orthogonal vectors $q_1, \ldots, q_k \in e^\perp$ such that*

$$-\frac{1}{2}A = \lambda ee^t + ez^t + ze^t + \sum_{j=1}^{k} q_j q_j^t, \tag{2.1.8}$$

where

$$\lambda = -\frac{1}{n}\sum_{j=1}^{k} q_j^t q_j \tag{2.1.9}$$

and z is determined by (2.1.8), (2.1.9), and the fact that A is hollow.

Proof It suffices to prove that (2.1.8)–(2.1.9) is equivalent to (c). Suppose that there exist mutually orthogonal vectors $q_1, \ldots, q_k \in e^\perp$ for which (2.1.8) holds. Extend $e/\sqrt{n}, q_1, \ldots, q_k$ to an orthogonal basis $e/\sqrt{n}, q_1, \ldots, q_{n-1}$ and let $Q = (q_1 \cdots q_{n-1})$. Then

$$Q^t\left(-\frac{1}{2}A\right)Q = Q^t\left(\sum_{j=1}^{k} q_j q_j^t\right)Q = \sum_{j=1}^{k}\left(Q^t q_j\right)\left(Q^t q_j\right)^t$$

is positive semidefinite of rank k, which is equivalent to (c).

Conversely, suppose that (c) holds for a specified U, in which case there exist mutually orthogonal vectors $w_1, \ldots, w_k \in e^\perp$ such that

$$-\frac{1}{2}U^t A U = \sum_{j=1}^{k} w_j w_j^t = WW^t.$$

Then

$$V^t\left(-\frac{1}{2}A\right)V = \begin{pmatrix} e^t/\sqrt{n} \\ U^t \end{pmatrix}\left(-\frac{1}{2}A\right)\begin{pmatrix} \frac{e}{\sqrt{n}} & U \end{pmatrix} = \begin{pmatrix} \nu & y^t \\ y & WW^t \end{pmatrix},$$

so

$$\nu + \text{trace}\left(WW^t\right) = \text{trace}\left(-\frac{1}{2}A\right) = 0$$

and

$$\begin{aligned} -\frac{1}{2}A &= VV^t\left(-\frac{1}{2}A\right)VV^t = \begin{pmatrix} \frac{e}{\sqrt{n}} & U \end{pmatrix}\begin{pmatrix} \nu & y^t \\ y & WW^t \end{pmatrix}\begin{pmatrix} e^t/\sqrt{n} \\ U^t \end{pmatrix} \\ &= \frac{\nu}{n}ee^t + e\frac{y^tU^t}{\sqrt{n}} + \frac{Uy}{\sqrt{n}}e^t + UWW^tU^t. \end{aligned}$$

Now let $\lambda = \nu/n$, $z = Uy/\sqrt{n}$, and $q_j = Uw_j$. Then $q_1, \ldots, q_k \in e^\perp$,

$$UWW^tU^t = U\left(\sum_{j=1}^k w_jw_j^t\right)U^t = \sum_{j=1}^k Uw_jw_j^tU^t = \sum_{j=1}^k q_jq_j^t,$$

and

$$\begin{aligned} \lambda = -\frac{1}{n}\text{trace}\left(WW^t\right) &= -\frac{1}{n}\text{trace}\left(W^tW\right) = -\frac{1}{n}\sum_{j=1}^k w_j^tw_j \\ &= -\frac{1}{n}\sum_{j=1}^k w_j^tU^tUw_j = -\frac{1}{n}\sum_{j=1}^k q_j^tq_j. \end{aligned}$$

□

We have not discovered our condition (d) in the literature. This is not surprising: the equivalence of (c) and (d) is trivial, and (c) is the more elegant condition. The importance of (d) is that it involves the Cayley-Menger matrix A_0. One can then use the interlacing inequalities to establish a direct connection between condition (c) and the classical condition (f) involving Cayley-Menger determinants, thereby strengthening our conviction that (c) is fundamental to understanding ESD matrices.

This connection interpolates condition (e), previously noted by Hayden and Wells [21, Theorem 3.1]. From (c) and (e), we can easily deduce the possible ranks of an ESD matrices.

Corollary 2.4 (Gower [19]) *If $A \in \mathcal{D}(n)$ and A has embedding dimension k, then* $\operatorname{rank}(A)$ *equals* $k+1$ *or* $k+2$.[6]

Proof It follows from (c) that U^tAU has k negative eigenvalues. Because U^tAU is a submatrix of V^tAV, it follows from the interlacing inequalities that V^tAV, hence A, has at least k negative eigenvalues. Furthermore, because $\operatorname{trace}(A) = 0$, A has at least one positive eigenvalue. Hence, $\operatorname{rank}(A)$ is at least $k+1$. Finally, it follows from (e) that $\operatorname{rank}(A_0) = k+2$. Because A is a submatrix of A_0, $\operatorname{rank}(A)$ is at most $k+2$. □

Each of the conditions in Theorem 2.1 specifies the embedding dimension of the distance matrix. Alternatively, the set of all ESD matrices can be characterized through a connection to the set of correlation matrices. The following characterization is noted in [13, p. 535], as a corollary of an elegant but complicated general theory of cuts and metrics. Here we provide a direct proof, again relying on condition (c).

Corollary 2.5 (Deza and Laurent [13]) *Let $\mathcal{E}(n)$ denote the set of $n \times n$ correlation matrices, i.e., symmetric positive semidefinite matrices with diagonal e, and let*

[6] Gower [19, Theorem 6] distinguished the two cases by demonstrating that $\operatorname{rank}(A) = k+1$ if and only if the points that generate A lie on a sphere. We derive a different characterization in Corollary 2.6.

$\mathcal{K}(n)$ denote the closure of the set

$$\left\{\lambda\left(ee^t - C\right) : \lambda \geq 0,\, C \in \mathcal{E}(n)\right\}.$$

Then $\mathcal{K}(n) = \mathcal{D}(n)$.

Proof To show that $\mathcal{K}(n) \subset \mathcal{D}(n)$, we suppose that $C = (c_{ij})$ is a correlation matrix and that $\lambda \geq 0$. Then C is positive definite and $c_{ii} = 1$, so $|c_{ij}| \leq 1$ and $ee^t - C$ is a pre-distance matrix. Furthermore, if U is any $n \times (n-1)$ matrix whose columns lie in $e^{\perp}$, then

$$U^t\left[\lambda\left(ee^t - C\right)\right]U = -\lambda U^t C U$$

is negative semidefinite. Applying condition (c) of Theorem 2.1, it follows that $\lambda(ee^t - C) \in \mathcal{D}(n)$. Then, because $\mathcal{D}(n)$ is closed, it must be that $\mathcal{K}(n) \subset \mathcal{D}(n)$.

To show that $\mathcal{D}(n) \subset \mathcal{K}(n)$, suppose that $A \in \mathcal{D}(n)$ has embedding dimension k. Given $\epsilon > 0$, we will demonstrate that there exists $\hat{A} \in \mathcal{D}(n)$ such that $\|\hat{A} - A\| \leq \epsilon$ and $\hat{A} \in \mathcal{K}(n)$. Because $\mathcal{K}(n)$ is closed, the desired inclusion will then follow.

First we construct $\hat{A}$. Let $x_1, \ldots, x_n$ be an e-centered spanning set of $\mathbf{R}^k$ for which $A = (\|x_i - x_j\|^2)$. By construction, the rows of the $k \times n$ matrix $X = (x_1 \cdots x_n)$ are linearly independent vectors in $e^{\perp}$. Choose $y_1, \ldots, y_n \in \mathbf{R}^{n-1-k}$ so that the rows of the $(n-1-k) \times n$ matrix $Y = (y_1 \cdots y_n)$ extend the rows of X to a basis for $e^{\perp}$. Let $A_y = (\|y_i - y_j\|^2)$. Given $\epsilon > 0$, let $\delta^2 = \epsilon / \|A_y\|$ and $z_i^t = (x_i^t, \delta y_i^t)$. Then $z_1, \ldots, z_n$ is an e-centered spanning set of $\mathbf{R}^{n-1}$ with ESD matrix

$$\hat{A} = \left(\|z_i - z_j\|^2\right) = \left(\|x_i - x_j\|^2\right) + \delta^2\left(\|y_i - y_j\|^2\right) = A + \delta^2 A_y,$$

and $\|\hat{A} - A\| = \delta^2 \|A_y\| = \epsilon$.

Next we show that $\hat{A} \in \mathcal{K}(n)$, i.e., that there exists $\lambda \geq 0$ such that $ee^t - \hat{A}/\lambda$ is a correlation matrix. Because $ee^t - \hat{A}/\lambda$ has unit diagonal entries for any λ, it suffices to find $\lambda \geq 0$ for which $ee^t - \hat{A}/\lambda$ is positive definite.

Again we apply condition (c) of Theorem 2.1. If U is such that $V = (\frac{e}{\sqrt{n}}|U)$ is orthogonal, then $U^t \hat{A} U$ is negative semidefinite. It follows that we can choose U so that $\Lambda = -U^t \hat{A} U$ is a diagonal matrix with nonnegative entries. For this choice of U,

$$
\begin{aligned}
ee^t - \frac{1}{\lambda}\hat{A} &= VV^t ee^t VV^t - \frac{1}{\lambda} VV^t \hat{A} VV^t \\
&= V \begin{pmatrix} n & 0 \\ 0 & 0 \end{pmatrix} V^t - \frac{1}{\lambda} V \begin{pmatrix} \frac{1}{n} e^t \hat{A} e & \frac{1}{\sqrt{n}} e^t \hat{A} U \\ \frac{1}{\sqrt{n}} U^t \hat{A} e & \Lambda \end{pmatrix} V^t \\
&= V \begin{pmatrix} n - \frac{1}{\lambda n} e^t \hat{A} e & -\frac{1}{\lambda\sqrt{n}} e^t \hat{A} U \\ -\frac{1}{\lambda\sqrt{n}} U^t \hat{A} e & \frac{1}{\lambda}\Lambda \end{pmatrix} V^t
\end{aligned}
$$

is obviously positive definite for sufficiently large $\lambda > 0$. □

Recently, Alfakih and Wolkowicz [2, Theorem 3.3] used Gale transforms to characterize those ESD matrices that can be represented as $A = \lambda(ee^t - C)$. The following result elaborates on their characterization; furthermore, it allows us to distinguish between ESD matrices of ranks $k+1$ and $k+2$. Notice that, if V is the orthogonal matrix constructed in the proof of Corollary 2.5, then

$$V^tAV = \left(\begin{array}{c|ccc|ccc} b_0 & b_1 & \cdots & b_k & b_{k+1} & \cdots & b_{n-1} \\ \hline b_1 & \lambda_1 & & & & & \\ \vdots & & \ddots & & & 0 & \\ b_k & & & \lambda_k & & & \\ \hline b_{k+1} & & & & & & \\ \vdots & & 0 & & & 0 & \\ b_{n-1} & & & & & & \end{array}\right). \tag{2.1.10}$$

Corollary 2.6 *Suppose that $A \in \mathcal{D}(n)$ has embedding dimension k and that $V = (\frac{e}{\sqrt{n}}|U)$ is an orthogonal matrix for which (2.1.10) is obtained. Then the following are equivalent:*

(a) There exist $\lambda \geq 0$ and $C \in \mathcal{E}(n)$ such that $A = \lambda(ee^t - C)$.

(b) $b_{k+1} = \cdots = b_{n-1} = 0$.

(c) $\text{rank}(A) = k + 1$.

Proof Because $\Lambda = U^tAU$ is negative semidefinite of rank k, thus $\lambda_1, \ldots, \lambda_k < 0$.

(a) ⇒ (b) Writing $C = ee^t - A/\lambda$, it follows from (2.1.10) that

$$V^tCV = \frac{1}{\lambda}\left(\begin{array}{c|ccc|ccc} \lambda n - b_0 & -b_1 & \cdots & -b_k & -b_{k+1} & \cdots & -b_{n-1} \\ \hline -b_1 & -\lambda_1 & & & & & \\ \vdots & & \ddots & & & 0 & \\ -b_k & & & -\lambda_k & & & \\ \hline -b_{k+1} & & & & & & \\ \vdots & & 0 & & & 0 & \\ -b_{n-1} & & & & & & \end{array}\right). \tag{2.1.11}$$

Because C, hence V^tCV, is positive semidefinite, so are the principal submatrices

$$\begin{pmatrix} \lambda n - b_0 & -b_i \\ -b_i & 0 \end{pmatrix},$$

which necessitates $b_i = 0$ for $i = k+1, \ldots, n-1$.

(b) ⇒ (a) Conversely, if $b_{k+1} = \cdots = b_{n-1} = 0$, then we can choose λ sufficiently large that the matrix in (2.1.11) is positive semidefinite. It follows that $C = ee^t - A/\lambda$ is a correlation matrix.

(b) ⇔ (c) Let L denote the leading $(k+1) \times (k+1)$ principal submatrix of V^tAV. Because $\lambda_1, \ldots, \lambda_k < 0$, L has at least k negative eigenvalues. But trace(L) = trace(V^tAV) = trace(A) = 0, so $b_0 > 0$ and L must have a positive eigenvalue. Thus, rank$(L) = k+1$ and rank(A) = rank$(V^tAV) \geq k+1$. It is obvious from the form of (2.1.10) that rank(A) = rank$(V^tAV) > k+1$ if and only if some $b_i \neq 0$, $i \in \{k+1, \ldots, n-1\}$. □

Alfakih and Wolkowicz [2] state condition (b) as $AZ = 0$, where Z is a *Gale matrix* associated with A. If $k = n-1$, then $Z = (0, \ldots, 0)^t$ and $AZ = 0$, while (b) is vacuously true. If $k < n-1$, then let $Z = (u_{k+1} \cdots u_{n-1})Q$, where $u_1, \ldots, u_{n-1}$ are the columns of U and Q is nonsingular. Then $U^tAZ = 0$ and, because the rows of U^t form a basis for $e^\perp$, the columns of AZ lie in the span of e. Hence, $AZ = 0$ if and only if $(b_{k+1}, \ldots, b_{n-1})^t = e^tAZ = 0$.

2.2 Consequences of the Characterizations of $\mathcal{D}(n)$

We proceed to exploit a well-known connection between $\mathcal{D}(n)$ and $\mathrm{PSD}(n-1)$, the subset of positive semidefinite matrices in $\mathbf{S}_{n-1}$. This connection follows immediately from our analysis of conditions (a), (b), and (c) in Theorem 2.1. The following notation is convenient: given $M \subset \mathbf{S}_m$, let $[M]$ denote the span of M in $\mathbf{S}_m$.

Given $w \in \mathbf{R}^n$ such that $e^tw \neq 0$, let $\mathcal{G}_w(n)$ denote the set of matrices of the form X^tX for some $k \times n$ matrix X that satisfies $Xw = 0$. The mapping $\tau_w : \mathbf{S}_n \to \mathbf{S}_n$ was defined by (2.1.1). Restricting its domain to $[\mathcal{D}(n)]$, we obtain the mapping $\tau_w : [\mathcal{D}(n)] \to [\mathcal{G}_w(n)]$. Similarly, the mapping $\kappa : \mathbf{S}_n \to \mathbf{S}_n$ was defined by (2.1.3). Restricting its domain to $[\mathcal{G}_w(n)]$, we obtain the mapping $\kappa : [\mathcal{G}_w(n)] \to [\mathcal{D}(n)]$. It is easily checked that these mappings are mutually inverse; see [12, 27] and our proof of the equivalence of conditions (a) and (b) in Theorem 2.1.

Let U be any $n \times (n-1)$ matrix for which the $n \times n$ matrix $V = (\frac{e}{\sqrt{n}}|U)$ is orthogonal. If $B = X^tX \in \mathcal{G}_w(n)$, then $U^tBU = (XU)^t(XU) \in \mathrm{PSD}(n-1)$. Hence,

$\psi_u(B) = U^tBU$ defines a linear mapping $\psi_u : [\mathcal{G}_w(n)] \to [\mathrm{PSD}(n-1)]$. Similarly, if $C = Y^tY \in \mathrm{PSD}(n-1)$, then $W^tCW = (YW)^t(YW) \in \mathcal{G}_w(n)$. Let $W = U^t(I - \frac{we^t}{e^tw})$. Then $\phi_u(C) = W^tCW$ defines a linear mapping $\phi_u : [\mathrm{PSD}(n-1)] \to [\mathcal{G}_w(n)]$. To see that ϕ_u and ψ_u are mutually inverse maps, first let $C \in [\mathrm{PSD}(n-1)]$. Because $WU = U^tU$ is the $(n-1)\times(n-1)$ identity matrix, $\psi_u \circ \phi_u(C) = U^tW^tCWU = C$, i.e., $\psi_u \circ \phi_u : [\mathrm{PSD}(n-1)] \to [\mathrm{PSD}(n-1)]$ is the identity map. Next let $B = X^tX \in \mathcal{G}_w(n)$, in which case $Xw = 0$. Recall, from the proof that (c) entails (b) in Theorem 2.1, that $UW = I - \frac{we^t}{e^tw}$. Then $XUW = X$ and $\phi_u \circ \psi_u(B) = W^tU^tX^tXUW = X^tX = B$. It follows that $\phi_u \circ \psi_u$ is the identity map on $\mathcal{G}_w(n)$, hence on $[\mathcal{G}_w(n)]$. Notice that both ψ_u and ϕ_u preserve rank.

Given w and U, let $\Psi = \psi_u \circ \tau_w$. Then $\Psi : [\mathcal{D}(n)] \to [\mathrm{PSD}(n-1)]$ is a linear bijection, and

$$\Psi(A) = -\frac{1}{2}U^t\left(I - \frac{ew^t}{e^tw}\right)A\left(I - \frac{we^t}{e^tw}\right)U = -\frac{1}{2}U^tAU$$

because $U^te = 0$. In what follows, we rely on Ψ to transfer well-known results and techniques from $\mathrm{PSD}(n-1)$ to $\mathcal{D}(n)$.

2.2.1 Facial structure of $\mathcal{D}(n)$

Following [47], a set $\mathcal{C}$ in a linear space $\mathcal{L}$ is *convex* if, for each $x, y \in \mathcal{C}$ and for all $\lambda \in [0,1]$, $\lambda x + (1-\lambda)y \in \mathcal{C}$. Furthermore, $\mathcal{C} \subset \mathcal{L}$ is a *convex cone* with vertex x_0 if it is a convex set and, for each $\lambda \geq 0$ and each $x \in \mathcal{C}$, $x \neq x_0$, we have $(1-\lambda)x_0 + \lambda x \in \mathcal{C}$.

Lemma 2.7 *$\mathcal{D}(n)$ is a convex cone.*

Proof We first show that $\mathcal{D}(n)$ is convex. Suppose that $A, B \in \mathcal{D}(n)$ and $\lambda \in [0,1]$. So $\Psi(A), \Psi(B) \in \mathrm{PSD}(n-1)$. By Theorem 2.1, $\lambda A + (1-\lambda)B \in \mathcal{D}(n)$ if and only if $\Psi(\lambda A + (1-\lambda)B) \in \mathrm{PSD}(n-1)$. Because $\mathrm{PSD}(n-1)$ is a convex cone and Ψ is linear, it follows that

$$\Psi(\lambda A + (1-\lambda)B) = \lambda\Psi(A) + (1-\lambda)\Psi(B) \in \mathrm{PSD}(n-1).$$

So $\mathcal{D}(n)$ is a convex cone. □

Again following [47], we say that a convex subset $\mathcal{F}$ of a convex set $\mathcal{C}$ is a *face* of $\mathcal{C}$ if and only if $x, y \in \mathcal{C}$ and $tx + (1-t)y \in \mathcal{F}$ for $t \in (0,1)$ implies $x, y \in \mathcal{F}$. Any convex set is a face of itself, and the intersection of any two faces is a face. The intersection of all faces of $\mathcal{C}$ that contain $a \in \mathcal{C}$ is the face *generated by* a. Various studies, e.g., [45, 3], have explored the facial structure of $\mathrm{PSD}(n-1)$, and the following result is well-known.

Theorem 2.8 *A set of matrices,* $\mathcal{E}$, *is a face of* $\mathrm{PSD}(n-1)$ *if and only if there exists a* $k \times (n-1)$ *matrix* Y *of rank* k *such that*

$$\mathcal{E} = \mathcal{E}(Y) = \left\{ Y^t Q Y : Q \in \mathrm{PSD}(k) \right\}. \tag{2.2.12}$$

A matrix B *generates* $\mathcal{E}(Y)$ *if and only if* $B = Y^t Q Y$ *for an invertible* $Q \in \mathrm{PSD}(k)$.

The facial structure of $\mathcal{D}(n)$ was investigated by Hayden, Wells, Liu, and Tarazaga [23], who relied on Corollary 2.3. In contrast, the bijective linear mapping Ψ can be exploited to deduce the facial structure of $\mathcal{D}(n)$ directly from the facial structure of $\mathrm{PSD}(n-1)$. This yields a statement that is more accessible than Theorem 2.3 in [23].

Theorem 2.9 *Fix $w \in \mathbf{R}^n$ with $w^t e \neq 0$. A set of matrices, $\mathcal{F}$, is a face of $\mathcal{D}(n)$ if and only if there exists $\{x_1, \dots, x_n\}$, a w-centered spanning set of $\mathbf{R}^k$, such that*

$$\mathcal{F} = \mathcal{F}(x_1, \dots, x_n) = \left\{ \left(\|Sx_i - Sx_j\|^2 \right) : S \in \mathbf{R}^{k \times k} \right\}. \tag{2.2.13}$$

A matrix B generates $\mathcal{F}(x_1, \dots, x_n)$ if and only if there exists $S \in \mathbf{R}^{k\times k}$ such that $B = (\|Sx_i - Sx_j\|^2)$ and $S^t S$ is invertible.

Proof The linear mapping Ψ is bijective, so $\mathcal{F}$ is a face of $\mathcal{D}(n)$ if and only if $\mathcal{E} = \Psi(\mathcal{F})$ is a face of PSD$(n-1)$. Hence, by Theorem 2.8, $\mathcal{F}$ is a face of $\mathcal{D}(n)$ if and only if there exists a $k \times (n-1)$ matrix Y of rank k such that $\Psi(\mathcal{F}) = \mathcal{E}(Y)$.

If $x_1, \dots, x_n$ is a w-centered spanning set of $\mathbf{R}^k$, then

$$\left(\|Sx_i - Sx_j\|^2 \right) = \left(x_i^t S^t S x_i - 2x_i S^t S x_j + x_j^t S^t S x_j \right) = JD - 2X^t S^t S X + DJ,$$

where $D = \text{diag}(x_1^t S^t S x_1, \dots, x_n^t S^t S x_n)$. Noting that $U^t J = JU = 0$, it follows that

$$\Psi\left(\left(\|Sx_i - Sx_j\|^2 \right) \right) = U^t X^t S^t S X U.$$

Suppose that $\mathcal{F} = \mathcal{F}(x_1, \dots, x_n)$, where $\{x_1, \dots, x_n\}$ is a w-centered spanning set of $\mathbf{R}^k$. To show that $\mathcal{F}$ is a face, write $X = (x_1 \cdots x_n)$ and let $Y = XU$. We claim that $\Psi(\mathcal{F}) = \mathcal{E}(Y)$.

Given $A = (\|Sx_i - Sx_j\|^2) \in \mathcal{F}$, let $Q = S^t S \in \text{PSD}(k)$. Then

$$\Psi(A) = U^t X^t S^t S X U = Y^t Q Y \in \mathcal{E}(Y),$$

so $\Psi(\mathcal{F}) \subset \mathcal{E}(Y)$. Conversely, given $Y^t Q Y \in \mathcal{E}(Y)$, write $Q = S^t S$. Then

$$Y^t Q Y = U^t X^t S^t S X U = \Psi\left(\left(\|Sx_i - Sx_j\|^2 \right) \right) \in \Psi(\mathcal{F}),$$

so $\mathcal{E}(Y) \subset \Psi(\mathcal{F})$.

Now suppose that $\mathcal{F}$ is a face of $\mathcal{D}(n)$, in which case $\Psi(\mathcal{F}) = \mathcal{E}(Y)$. As in the proof that (c) implies (b) in Theorem 2.1, let $X = YU^t(I - \frac{we^t}{e^tw})$ and let $x_1, \ldots, x_n$ denote the columns of X, a w-centered spanning set of $\mathbf{R}^k$. Notice that $U^t(I - \frac{we^t}{e^tw})U = I$, hence that $XU = Y$. We claim that $\mathcal{F} = \mathcal{F}(x_1, \ldots, x_n)$.

Given $A = (\|Sx_i - Sx_j\|^2) \in \mathcal{F}(x_1, \ldots, x_n)$, let $Q = S^tS \in \mathrm{PSD}(k)$. Then

$$\Psi(A) = U^tX^tS^tSXU = Y^tQY \in \mathcal{E}(Y),$$

so $\Psi(\mathcal{F}(x_1, \ldots, x_n)) \subset \mathcal{E}(Y)$ and therefore $\mathcal{F}(x_1, \ldots, x_n) \subset \mathcal{F}$. Conversely, given $A \in \mathcal{F}$, write $\Psi(A) = Y^tQY$ and $Q = S^tS$. Then

$$Y^tQY = U^tX^tS^tSXU = \Psi\left(\left(\|Sx_i - Sx_j\|^2\right)\right) \in \Psi\left(\mathcal{F}\left(x_1, \ldots, x_n\right)\right),$$

so $\mathcal{E}(Y) \subset \Psi(\mathcal{F}(x_1, \ldots, x_n))$ and therefore $\mathcal{F} \subset \mathcal{F}(x_1, \ldots, x_n)$.

Finally, $A = (\|Sx_i - Sx_j\|^2)$ generates $\mathcal{F}(x_1, \ldots, x_n)$ if and only if $B = \Psi(A) = U^tX^tS^tSXU$ generates $\mathcal{E}(XU)$. By Theorem 2.8, B generates $\mathcal{E}(XU)$ if and only if $Q = S^tS$ is invertible. □

2.2.2 Angles between matrices in $\mathcal{D}(n)$

Given $A, B \in \mathrm{S}_m$, let $\langle A, B\rangle = \mathrm{trace}(A^tB)$ denote the Frobenius inner product of A and B. The corresponding Frobenius norm is defined by $\|A\|^2 = \langle A, A\rangle$, and the angle between A and B with respect to the Frobenius inner product, $\theta \in [0, \pi]$, is defined by

$$\cos\theta = \frac{\langle A, B\rangle}{\|A\|\,\|B\|} = \cos\left(A, B\right).$$

For example, all rank-one matrices $xx^t \in \mathrm{PSD}(m)$ have the same angle with the $m \times m$ identity matrix, I_m, because

$$\cos\left(xx^t, I_m\right) = \frac{\langle xx^t, I_m\rangle}{\|xx^t\| \ \|I_m\|} = \frac{x^t x}{\sqrt{(x^t x)^2}\sqrt{m}} = \frac{1}{\sqrt{m}}.$$

In their study of the geometry of $\mathcal{D}(n)$, Hayden, Wells, Liu, and Tarazaga [23] obtained upper and lower bounds on the angle between an arbitrary $A \in \mathcal{D}(n)$ of embedding dimension $k = 1$ and $E = ee^t - I_n \in \mathcal{D}(n)$. They deduced their upper bounds from their analysis of the critical points of the function $F : \mathbf{R}^n \to \mathbf{R}$ defined by

$$F(x_1, \ldots, x_n) = \left\|\left(|x_i - x_j|^2\right) - E\right\|^2.$$

Their analysis "is difficult and tedious," requiring "a difficult case by case analysis" not included in [23]. Here, we map $\mathcal{D}(n)$ to $\mathcal{G}_e(n)$, then infer bounds on $\cos(A, E)$ from properties of κ, appealing to results obtained by Critchley [12].

We require two technical lemmas. Lemma 2.10 restates Proposition 2.3 and Corollary 2.9 in [12]; we provide a proof of Lemma 2.11 in Section 2.2.4.

Lemma 2.10 (Critchley [12]) *The linear subspaces*

$$\begin{aligned}
\mathcal{S}_1 &= \{B \in \mathcal{G}_e(n) : B \circ I = 0\} \\
\mathcal{S}_2 &= \left\{B \in \mathcal{G}_e(n) : B = we^t + ew^t - nwe^t \circ I, w^t e = 0\right\} \\
\mathcal{S}_3 &= \left\{B \in \mathcal{G}_e(n) : B = \gamma\left(I - \frac{ee^t}{n}\right), \gamma \in \mathbf{R}\right\},
\end{aligned}$$

are pairwise orthogonal and have direct sum $\mathcal{G}_e(n)$. The linear subspaces $\kappa(\mathcal{S}_1)$, $\kappa(\mathcal{S}_2)$, *and $\kappa(S_3)$ are pairwise orthogonal and have direct sum $\mathcal{D}(n)$. Furthermore,*

$$\|\kappa(B)\| = \left\{ \begin{array}{ll} 2\|B\| & \text{if } B \in S_1 \\ \sqrt{2n}\|B\| & \text{if } B \in S_2 \\ 2\sqrt{n}\|B\| & \text{if } B \in S_3 \end{array} \right\}.$$

Lemma 2.11 *For $n \geq 2$, write $x = (x_1, \ldots, x_n)^t$ and define $f : \mathbf{R}^n \to \mathbf{R}$ by $f(x) = x_1^4 + \cdots + x_n^4$. Let $K_n = \{x \in \mathbf{R}^n : x^t x = 1, x^t e = 0\}$. If $x \in K_n$, then*

$$\frac{n^2 - 3n + 3}{n\,(n-1)} \geq f(x) \geq \left\{ \begin{array}{ll} \frac{n^2+3}{n(n-1)(n+1)} & \text{for } n \text{ odd} \\ \frac{1}{n} & \text{for } n \text{ even} \end{array} \right\}. \tag{2.2.14}$$

The upper bound is obtained if and only if a permutation of $(x_1, \ldots, x_n)$ equals

$$\pm(a, \underbrace{b, \ldots, b}_{n-1}),$$

where $a = (n-1)/\sqrt{n(n-1)}$ and $b = -1/\sqrt{n(n-1)}$. The lower bound is obtained if and only if a permutation of $(x_1, \ldots, x_n)$ equals

$$\pm(\underbrace{a, \ldots, a}_{\lfloor n/2 \rfloor}, \underbrace{b, \ldots, b}_{\lceil n/2 \rceil}),$$

where $a = -b = 1/\sqrt{n}$ if n is even and

$$(a, b) = \left(\sqrt{\frac{n+1}{n(n-1)}}, -\sqrt{\frac{n-1}{n(n+1)}} \right)$$

if n is odd.

Now we bound $\cos(A, E)$. We obtain the upper bounds in [23]; for $n \geq 4$, we obtain sharper lower bounds.

Theorem 2.12 *For $n \geq 2$, let $E = ee^t - I$ and suppose that $A \in \mathcal{D}(n)$ has embedding dimension $k = 1$. Then*

$$\frac{4n}{(n-1)(n+6)} \leq [\cos(A,E)]^2 \leq \left\{ \begin{array}{ll} \frac{n}{2(n-1)} & \text{for } n \text{ even} \\ \frac{n+1}{2n} & \text{for } n \text{ odd} \end{array} \right\}.$$

Proof From condition (b) in Theorem 2.1, there exists $x = (x_1, \ldots, x_n)^t \in \mathbf{R}^n$ such that $x^t e = 0$ and $\tau_e(A) = xx^t$. Because $\cos(A, E)$ is invariant under dilations of A, we can assume that $x^t x = 1$.

Applying Lemma 2.10, we write $xx^t = \alpha B_1 + \beta B_2 + \gamma B_3$ for some $B_1 \in \mathcal{S}_1$, $B_2 \in \mathcal{S}_2$, and $B_3 = I - \frac{ee^t}{n}$. Because $x^t x = 1$, $1 = \|\alpha B_1\|^2 + \|\beta B_2\|^2 + \|\gamma B_3\|^2$.

Because $\|B_3\|^2 = n - 1$,

$$\gamma(n-1) = \langle xx^t, B_3 \rangle = \text{trace}\left(\left(xx^t\right)^t \left(I - \frac{ee^t}{n}\right)\right) = \text{trace}\left(xx^t\right) = 1.$$

Hence, $\gamma = 1/(n-1)$ and $\|\gamma B_3\|^2 = 1/(n-1)$.

By direct calculation,

$$\|B_2\|^2 = \text{trace}\left(\left[we^t + ew^t - nwe^t \circ I\right]^t \left[we^t + ew^t - nwe^t \circ I\right]\right) = n(n-2)w^t w.$$

Because $\text{diag}(B_1) = 0$, $\text{diag}(B_2) = \text{diag}(we^t + ew^t - nwe^t \circ I) = (2-n)w$, and $\text{diag}(B_3) = (n-1)e/n$,

$$\beta(2-n)w = \text{diag}(\beta B_2) = \text{diag}(\alpha B_1 + \beta B_2) = \text{diag}\left(xx^t - \gamma B_3\right) = \begin{pmatrix} x_1^2 \\ \vdots \\ x_n^2 \end{pmatrix} - \frac{e}{n}.$$

Hence,

$$\|\beta B_2\|^2 = \beta^2 n(n-2)w^t w = \frac{n}{n-2}\left[\beta(2-n)w\right]^t\left[\beta(2-n)w\right] = \frac{n}{n-2}\left[\sum_{i=1}^n x_i^4 - \frac{1}{n}\right].$$

Now we write $A = \kappa(xx^t)$. We calculate that $\tau_e\left(ee^t - I\right) = \frac{1}{2}(I - \frac{ee^t}{n})$ and write $E = \kappa(B_3/2)$. Then

$$\begin{aligned}
\frac{\langle A, E\rangle}{\|A\|\;\|E\|} &= \frac{\langle \alpha\kappa(B_1) + \beta\kappa(B_2) + \gamma\kappa(B_3), \frac{1}{2}\kappa(B_3)\rangle}{\left(\|\kappa(\alpha B_1)\|^2 + \|\kappa(\beta B_2)\|^2 + \|\kappa(\gamma B_3)\|^2\right)^{1/2}\;\frac{1}{2}\|\kappa(B_3)\|} \\
&= \frac{\gamma\|\kappa(B_3)\|^2}{\left(4\|\alpha B_1\|^2 + 2n\|\beta B_2\|^2 + 4n\|\gamma B_3\|^2\right)^{1/2}\;\|\kappa(B_3)\|} \\
&= \frac{2\sqrt{n}\|\gamma B_3\|}{\left(4 - 4\|\beta B_2\|^2 - 4\|\gamma B_3\|^2 + 2n\|\beta B_2\|^2 + 4n\|\gamma B_3\|^2\right)^{1/2}} \\
&= \frac{2\sqrt{n/(n-1)}}{\left(4 + 2n\left(\sum_{i=1}^n x_i^4 - \frac{1}{n}\right) + 4\right)^{1/2}} \\
&= \left(\frac{4n/(n-1)}{6 + 2n\sum_{i=1}^n x_i^4}\right)^{1/2}. \qquad (2.2.15)
\end{aligned}$$

To minimize/maximize $\cos(A, E)$, we maximize/minimize (2.2.15), i.e., we minimize/maximize $f(x) = \sum x_i^4$ subject to $x \in K$. Lemma 2.11 specifies the minimum and maximum values, which we substitute into (2.2.15) to conclude the proof. □

2.2.3 Linear preservers of $\mathcal{D}(n)$

One way to understand a set of matrices is by studying linear operators that preserve its structure [37]. We exploit the connection between $\mathcal{D}(n)$ and $\mathrm{PSD}(n-1)$ to study linear operators that preserve the faces of $\mathcal{D}(n)$.

We begin by characterizing the linear operators that preserve the faces of $\mathrm{PSD}(n-1)$.

Theorem 2.13 *Let* $K = \{k_1, \ldots, k_m\} \neq \{0\}$ *be such that* $0 \leq k_1 < \ldots < k_m \leq n-1$. *Let*

$$\mathcal{C} = \{C \in \mathrm{PSD}(n-1) : \mathrm{rank}(C) \in K\}. \tag{2.2.16}$$

Then a linear operator $T : \mathrm{S}_{n-1} \to \mathrm{S}_{n-1}$ *preserves* $\mathcal{C}$*, i.e.,* $T(\mathcal{C}) = \mathcal{C}$*, if and only if there exists an invertible matrix* R *such that* $T(C) = R^tCR$.

Proof If $T(C) = R^tCR$ with R invertible, then it follows from Sylvester's Law of Inertia that $T(\mathcal{C}) = \mathcal{C}$. It remains to establish the converse. Let

$$\mathcal{C}_j = \{C \in \mathrm{PSD}(n-1) : \mathrm{rank}(C) = j\} \quad \text{and} \quad \hat{\mathcal{C}}_k = \bigcup_{j=0}^{k} \mathcal{C}_j.$$

We claim that $\hat{\mathcal{C}}_k = \mathrm{cl}(\mathcal{C}_k)$, the closure of $\mathcal{C}_k$.

Because $\mathcal{C}_k \subset \hat{\mathcal{C}}_k$ and $\hat{\mathcal{C}}_k$ is closed, $\mathrm{cl}(\mathcal{C}_k) \subset \hat{\mathcal{C}}_k$. If $C \in \mathcal{C}_k$, then obviously $C \in \mathrm{cl}(\mathcal{C}_k)$. If $C \in \mathcal{C}_j$ for $j < n$, then write $C = Y_j^tY_j$ for a $j \times (n-1)$ matrix Y_j. Let Y_{k-j} be any $(k-j) \times (n-1)$ matrix such that $(Y_j^t|Y_{k-j}^t)$ has rank k, let $c = 1/\|Y_{k-j}^tY_{k-j}\|$, and let $C_i = Y_j^tY_j + (c/i)Y_{k-j}^tY_{k-j}$. Then $C_i \in \mathcal{C}_k$ and $\|C_i - C\| = c/i \to 0$ as $i \to \infty$, so each $C \in \hat{\mathcal{C}}_k$ is the limit point of a sequence in $\hat{\mathcal{C}}_k$. This proves that $\hat{\mathcal{C}}_k \subset \mathrm{cl}(\mathcal{C}_k)$. It also demonstrates that $\mathrm{int}(\hat{\mathcal{C}}_k)$, the relative interior of $\hat{\mathcal{C}}_k$, is contained in $\mathcal{C}_k$. Because $\mathcal{C}_k$ is open in $\hat{\mathcal{C}}_k$, $\mathrm{int}(\hat{\mathcal{C}}_k) = \mathcal{C}_k$.

Now suppose that $T(\mathcal{C}) = \mathcal{C}$. Because T is continuous,

$$T\left(\hat{\mathcal{C}}_{k_m}\right) = T\left(\mathrm{cl}\left(\mathcal{C}\right)\right) = \mathrm{cl}\left(\mathcal{C}\right) = \hat{\mathcal{C}}_{k_m}. \tag{2.2.17}$$

Because T is linear,

$$T\left(\mathcal{C}_{k_m}\right) = T\left(\mathrm{int}\left(\hat{\mathcal{C}}_{k_m}\right)\right) = \mathrm{int}\left(\hat{\mathcal{C}}_{k_m}\right) = \mathcal{C}_{k_m}. \tag{2.2.18}$$

Subtracting (2.2.18) from (2.2.17), we obtain

$$T\left(\hat{\mathcal{C}}_{k_m-1}\right) = T\left(\hat{\mathcal{C}}_{k_m} - \mathcal{C}_{k_m}\right) = T\left(\hat{\mathcal{C}}_{k_m}\right) - T\left(\mathcal{C}_{k_m}\right) = \hat{\mathcal{C}}_{k_m} - \mathcal{C}_{k_m} = \hat{\mathcal{C}}_{k_m-1}.$$

We continue to "peel the onion" in this manner, concluding that $T(\mathcal{C}_1) = \mathcal{C}_1$. It then follows from Theorem 3 in [24] that T is of the form $T(C) = \pm R^t C R$. Because C and $T(C)$ are positive semidefinite, we conclude that $T(C) = R^t C R$. □

Next we set $w = e$ and characterize the linear operators that preserve the faces of $\mathcal{G}_e(n)$.

Theorem 2.14 *Let $K = \{k_1, \ldots, k_m\} \neq \{0\}$ be such that $0 \leq k_1 < \ldots < k_m \leq n-1$. Let*

$$\mathcal{B} = \{B \in \mathcal{G}_e(n) : \text{rank}(B) \in K\}. \tag{2.2.19}$$

Then a linear operator $T : [\mathcal{G}_e(n)] \to [\mathcal{G}_e(n)]$ preserves $\mathcal{B}$, i.e., $T(\mathcal{B}) = \mathcal{B}$, if and only if there exists an $n \times n$ matrix Q, with rank$(Q) = n-1$ and $Qe = Q^t e = 0$, such that $T(B) = Q^t B Q$.

Proof Fix $w = e$ and U, any $n \times (n-1)$ matrix for which $(\frac{e}{\sqrt{n}}|U)$ is orthogonal. Then $W = U^t(I - \frac{ee^t}{n}) = U^t$, so $\psi_u(B) = U^t B U$ and $\phi_u(C) = W^t C W = U C U^t$.

Let $\mathcal{C} = \psi_u(\mathcal{B})$, in which case $\mathcal{B} = \phi_u(\mathcal{C})$. Then $T(\mathcal{B}) = \mathcal{B}$ if and only if $T \circ \phi_u(\mathcal{C}) = \phi_u(\mathcal{C})$ if and only if $\psi_u \circ T \circ \phi_u(\mathcal{C}) = \mathcal{C}$. Because ψ_u and ϕ_u preserve rank, $\mathcal{C} \subset \text{PSD}(n-1)$ is a set of the form (2.2.16); hence, it follows from Theorem 2.13 that $T(\mathcal{B}) = \mathcal{B}$ if and only if there exists an invertible matrix R such that $\psi_u \circ T \circ \phi_u(C) = R^t C R$.

Suppose that there exists an $(n-1)\times(n-1)$ invertible matrix R such that $\psi_u \circ T \circ \phi_u(C) = R^tCR$. Let $Q = URU^t$. Then $\text{rank}(Q) = n-1$, $Qe = Q^te = 0$, and

$$\begin{aligned} T(B) &= \phi_u \circ \psi_u \circ T \circ \phi_u \circ \psi_u(B) = \phi_u \circ \psi_u \circ T \circ \phi_u\left(U^tBU\right) \\ &= \phi_u\left(R^tU^tBUR\right) = UR^tU^tBURU^t = Q^tBQ. \end{aligned}$$

Conversely, suppose that there exists an $n\times n$ matrix Q such that $\text{rank}(Q) = n-1$, $Qe = Q^te = 0$, and $T(B) = Q^tBQ$. Let $R = U^tQU$. Then R is invertible and

$$\psi_u \circ T \circ \phi_u(C) = \psi_u \circ T\left(UCU^t\right) = \psi_u\left(Q^tUCU^tQ\right) = U^tQ^tUCU^tQU = R^tCR.$$

□

Finally, we characterize the linear operators that preserve the faces of $\mathcal{D}(n)$. Let $\dim(A)$ denote the embedding dimension of $A \in \mathcal{D}(n)$.

Theorem 2.15 *Let $K = \{k_1, \ldots, k_m\} \neq \{0\}$ be such that $0 \le k_1 < \ldots < k_m \le n-1$. Let*

$$\mathcal{A} = \{A \in \mathcal{D}(n) : \dim(A) \in K\}.$$

Then a linear operator $T : [\mathcal{D}(n)] \to [\mathcal{D}(n)]$ preserves $\mathcal{A}$, i.e., $T(\mathcal{A}) = \mathcal{A}$, if and only if there exists an $n\times n$ matrix Q, with $\text{rank}(Q) = n-1$ and $Qe = Q^te = 0$, such that $T(A) = -\kappa(Q^tAQ)/2$.

Proof Let $\mathcal{B} = \tau_e(\mathcal{A})$, in which case $\mathcal{A} = \kappa(\mathcal{B})$. Then $T(\mathcal{A}) = \mathcal{A}$ if and only if $T \circ \kappa(\mathcal{B}) = \kappa(\mathcal{B})$ if and only if $\tau_e \circ T \circ \kappa(\mathcal{B}) = \mathcal{B}$. Because of the equivalence of conditions (a) and (b) in Theorem 2.1, $\mathcal{B} \subset \mathcal{G}_e(n)$ is a set of the form (2.2.19); hence, it follows from Theorem 2.14 that $T(\mathcal{A}) = \mathcal{A}$ if and only if there exists an $n \times n$ matrix Q, with $\text{rank}(Q) = n-1$ and $Qe = Q^te = 0$, such that

$$\tau_e \circ T \circ \kappa(B) = Q^tBQ. \tag{2.2.20}$$

Now we apply κ to both sides of (2.2.20), obtaining

$$\begin{aligned} T(A) &= T \circ \kappa(B) = \kappa\left(Q^tBQ\right) = \kappa\left(Q^t\tau_e(A)Q\right) \\ &= -\frac{1}{2}\kappa\left(Q^t\left(I - \frac{ee^t}{n}\right)A\left(I - \frac{ee^t}{n}\right)Q\right) = -\frac{1}{2}\kappa\left(Q^tAQ\right). \end{aligned}$$

□

2.2.4 Proof of Lemma 2.11

We conclude with a proof of Lemma 2.11, which relies on two simple facts.

Lemma 2.16 *Suppose that $\alpha, \beta, \gamma \in \mathbf{R}$ and $\alpha + \beta + \gamma = 0$. Then*

$$\alpha^4 + \beta^4 + \gamma^4 = \frac{1}{2}\left(\alpha^2 + \beta^2 + \gamma^2\right)^2.$$

Proof of Lemma 2.16 Let $a = \alpha/2$ and $b = \beta + a$. Then

$$\begin{aligned} \alpha^4 + \beta^4 + \gamma^4 &= (2a)^4 + (-a+b)^4 + (-a-b)^4 = 18a^4 + 12a^2b^2 + 2b^4; \\ \left(\alpha^2 + \beta^2 + \gamma^2\right)^2 &= \left((2a)^2 + (-a+b)^2 + (-a-b)^2\right)^2 \\ &= \left(6a^2 + 2b^2\right)^2 = 36a^4 + 24a^2b^2 + 4b^4. \end{aligned}$$

□

Lemma 2.17 *Suppose that the cubic equation $x^3 - ax - b = 0$ has roots α, β, γ. Then $\alpha + \beta + \gamma = 0$ and $\alpha^2 + \beta^2 + \gamma^2 = 2a$.*

Proof of Lemma 2.17 Writing

$$\begin{aligned} x^3 - ax - b &= (x-\alpha)(x-\beta)(x-\gamma) \\ &= x^3 - (\alpha+\beta+\gamma)x^2 + (\alpha\beta+\beta\gamma+\alpha\gamma)x - \alpha\beta\gamma, \end{aligned}$$

we see that $\alpha+\beta+\gamma=0$ and $\alpha\beta+\beta\gamma+\alpha\gamma=-a$. It follows that

$$\alpha^2+\beta^2+\gamma^2-2a = \alpha^2+\beta^2+\gamma^2+2(\alpha\beta+\beta\gamma+\alpha\gamma) = (\alpha+\beta+\gamma)^2 = 0.$$

□

Proof of Lemma 2.11 If $n=2$ and $x \in K_2$, then it is easily verified that $f(x) = 1/2$, the value of both the upper and lower bounds.

If $n=3$ and $x=(\alpha,\beta,\gamma)^t \in K_3$, then it follows from Lemma 2.16 that $f(x)=1/2$, the value of both the upper and lower bounds.

Suppose that $n \geq 4$. Because f is continuous and K_n is compact, f attains both a maximum and minimum in K_n. If x^* is a constrained maximizer or minimizer of f, then there exist Lagrange multipliers λ^* and μ^* such that (x^*,λ^*,μ^*) is a stationary point of the Lagrangian function

$$L(x_1,\ldots,x_n,\lambda,\mu) = \left(x_1^4+\cdots+x_n^4\right) + \lambda\left(x_1^2+\cdots+x_n^2-1\right) + \mu\left(x_1+\cdots+x_n\right),$$

i.e., each x_i^* is a solution of the cubic equation

$$4x^3 - 2\lambda^* x - \mu^* = 0. \tag{2.2.21}$$

Because $x^* \in K_n$, the x_i^* must assume more than one value. Because the x_i^* are roots of a cubic polynomial, they can assume at most three values. We claim that they assume exactly two values.

Suppose that the x_i^* assume three distinct values, α, β, γ. Then α, β, γ are the roots of (2.2.21), so it follows from Lemma 2.17 that $\alpha+\beta+\gamma=0$ and $\alpha^2+\beta^2+\gamma^2=\lambda^*$. Choose three more distinct values, $\hat{\alpha}, \hat{\beta}, \hat{\gamma}$, such that $\hat{\alpha}+\hat{\beta}+\hat{\gamma}=0$, $\hat{\alpha}^2+\hat{\beta}^2+\hat{\gamma}^2=\lambda^*$, and $\hat{\alpha}, \hat{\beta}, \hat{\gamma} \notin \{\alpha, \beta, \gamma\}$. It follows from Lemma 2.16 that $\alpha^4+\beta^4+\gamma^4=(\lambda^*)^2/2$ and $\hat{\alpha}^4+\hat{\beta}^4+\hat{\gamma}^4=(\lambda^*)^2/2$.

To simplify notation, suppose that $(x_1^*, x_2^*, x_3^*) = (\alpha, \beta, \gamma)$ and let

$$\hat{x} = (\hat{\alpha}, \hat{\beta}, \hat{\gamma}, x_4^*, \ldots, x_n^*)^t.$$

Then

$$\begin{aligned}
\hat{\alpha}+\hat{\beta}+\hat{\gamma}+\sum_{i=1}^{n} x_i^* &= \alpha+\beta+\gamma+\sum_{i=4}^{n} x_i^* = 0, \\
\hat{\alpha}^2+\hat{\beta}^2+\hat{\gamma}^2+\sum_{i=1}^{n} (\hat{x}_i)^2 &= \alpha^2+\beta^2+\gamma^2+\sum_{i=4}^{n} (x_i^*)^2 = 1, \\
\hat{\alpha}^4+\hat{\beta}^4+\hat{\gamma}^4+\sum_{i=1}^{n} (\hat{x}_i)^4 &= \alpha^4+\beta^4+\gamma^4+\sum_{i=4}^{n} (x_i^*)^4,
\end{aligned}$$

so $\hat{x} \in K_n$ and $f(\hat{x}) = f(x^*)$. Hence, if x^* is an extreme point of f in K_n, then so is $\hat{x}$. But the $\hat{x}_i$ assume at least four distinct values, which an extreme point of f in K_n cannot. We conclude that the x_i^* cannot assume more than two distinct values.

Suppose that k of the x_i^* equal α and the remaining $n-k$ of the x_i^* equal β, where α, β are chosen so that $0 < k \leq n/2$. Because $0 = x_1^* + \cdots + x_n^* = k\alpha + (n-k)\beta$, $\beta = -k\alpha/(n-k)$ and therefore

$$1 = \sum_{i=1}^{n} (x_i^*)^2 = k\alpha^2 + (n-k)\beta^2 = k\alpha^2 + \frac{k^2}{n-k}\alpha = \frac{nk}{n-k}\alpha^2.$$

It follows that $\alpha^2 = (n-k)/(nk)$ and $\beta^2 = k/(n(n-k))$, and therefore

$$\begin{aligned} f(x^*) &= \sum_{i=1}^{n} (x_i^*)^2 = k\alpha^4 + (n-k)\beta^4 = k\left(\frac{n-k}{nk}\right)^2 + (n-k)\left(\frac{k}{n(n-k)}\right)^2 \\ &= \frac{n^2-3kn+3k^2}{nk(n-k)} = \frac{(n-2k)^2}{nk(n-k)} + \frac{1}{n}. \end{aligned} \quad (2.2.22)$$

By inspection, (2.2.22) is maximal when $k=1$ and minimal when $k=[n/2]$, yielding the specified bounds. □

2.3 Uniqueness of Completions

In this section, we will give a brief introduction to the study of completion problems and to our problem in particular. This problem, can be generalized to a problem about PSD matrices. Using this generalization, we first obtain a necessary and sufficient condition for an $n \times n$ partial matrix A to have a unique positive semi-definite completion. We then use the result to deduce the conditions for the uniqueness of the ESD matrix completion. We also show how it is useful in the contractive matrix completion problem. (Recall that a matrix is contractive if its operator norm is at most one.) Furthermore, we describe an algorithm to check the conditions in our results, and how to use existing software to check the conditions numerically. At the end of the section, we illustrate our results by several numerical examples, and show that some results in [1] are not accurate.

2.3.1 Completion problems

In the study of completion problems, one considers a partially specified matrix and tries to fill in the missing entries so that the resulting matrix has some specific properties such as being invertible, having a specific rank, being positive semi-definite, etc. One can ask the following general problems:

(a) Determine whether a completion with the desired property exists.

(b) Determine all completions with the desired property.

(c) Determine whether there is a unique completion with the desired property.

See [26] for general background of completion problems.

In [1], the author raised the problem of determining the condition on an $n \times n$ partial matrix A under which there is a unique way to complete it to an ESD matrix. In this section, we give a complete answer to this problem. It turns out that the desired uniqueness condition can be determined by the existence of a positive semi-definite matrix satisfying certain linear constraints. Such a condition can be checked by existing computer software such as the semi-definite programming routines; see [29, 49].

2.3.2 A general formulation

In the following discussion, we will consider problems in the following more general settings.

Let $\mathcal{M}$ be a matrix space, and $\mathcal{S}$ a subspace of $\mathcal{M}$. Suppose $\mathcal{P}$ is a subset of $\mathcal{M}$ with certain desirable properties. Given $A \in \mathcal{M}$, we would like to determine $X \in \mathcal{S}$ so that

$$A + X \in \mathcal{P}.$$

In our case, we are interested in the condition for the uniqueness of $X \in \mathcal{S}$ such that $A + X \in \mathcal{P}$.

To recover the completion problem, suppose a partial matrix is given. Let A be an arbitrary completion of the partial matrix, say, set all unspecified entries to 0. Let $\mathcal{S}$ be the space of matrices with zero entries at the specified entries of the given partial matrix. Suppose $\mathcal{P}$ is a subset of $\mathcal{M}$ with the desired property such as being invertible, having a specific rank, being positive semi-definite, etc. Then completing the partial matrix to a matrix in $\mathcal{P}$ is the same as finding $X \in \mathcal{S}$ such that $A+X \in \mathcal{P}$.

In the following, we always assume that there is an $X_0 \in \mathcal{S}$ such that $A+X_0 \in \mathcal{P}$, and study the condition under which X_0 is the only matrix in $\mathcal{S}$ satisfying $A+X_0 \in \mathcal{P}$. We can always assume that $X_0 = 0$ by replacing A by $A + X_0$.

We begin with the following result concerning the uniqueness of the positive semi-definite completion problem.

Proposition 2.18 *Let $A \in \mathrm{PSD}(n)$, and $\mathcal{S}$ be a subspace of S_n. Suppose V is orthogonal such that $V^tAV = \mathrm{diag}\,(d_1, \dots, d_r, 0, \dots, 0)$, where $d_1 \geq \cdots \geq d_r > 0$. If $X \in \mathcal{S}$ satisfies $A + X \in \mathrm{PSD}(n)$, then*

$$V^tXV = \begin{pmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{pmatrix} \tag{2.3.23}$$

with

$$X_{22} \in \mathrm{PSD}(n-r) \quad \textit{and} \quad \mathrm{rank}\,(X_{22}) = \mathrm{rank}\,([X_{21}\ X_{22}]). \tag{2.3.24}$$

Conversely, if there is $X \in \mathcal{S}$ such that (2.3.23) *and* (2.3.24) *hold then there is an $\varepsilon > 0$ such that $A + \delta X \in \mathrm{PSD}(n)$ for all $\delta \in [0, \varepsilon]$.*

Proof. Suppose $A + P \in \mathrm{PSD}(n)$. Let $X = P$, and consider the block matrix V^tXV defined as in (2.3.23). We have $X_{22} \in \mathrm{PSD}(n-r)$ because

$$\begin{pmatrix} D + X_{11} & X_{12} \\ X_{21} & X_{22} \end{pmatrix} \in \mathrm{PSD}(n) \qquad \text{with } D = \mathrm{diag}\,(d_1, \ldots, d_r).$$

Let W be orthogonal such that $W^tX_{22}W = \mathrm{diag}\,(c_1, \ldots, c_s, 0, \ldots, 0)$ with $c_1 \geq \cdots \geq c_s > 0$. If $\widetilde{W} = I_r \oplus W$, then

$$\widetilde{W}^tV^t(A+P)V\widetilde{W} = \begin{pmatrix} D + X_{11} & Y_{12} \\ Y_{21} & W^tX_{22}W \end{pmatrix}.$$

Since $A + P \in \mathrm{PSD}(n)$, we see that only the first s rows of Y_{21} can be nonzero. Thus,

$$\mathrm{rank}\,([X_{21}\ X_{22}]) = \mathrm{rank}\,([Y_{21}\ W^tX_{22}W]) = s = \mathrm{rank}\,(X_{22}).$$

Conversely, suppose there is an $X \in \mathcal{S}$ such that (2.3.23) and (2.3.24) hold. Then for sufficiently large $\eta > 0$, $\eta D + X_{11}$ is positive definite. Moreover, if

$$T = \begin{pmatrix} I_r & -(\eta D + X_{11})^{-1}X_{12} \\ 0 & I_{n-r} \end{pmatrix},$$

then

$$T^tV^t(\eta A + X)VT = (\eta D + X_{11}) \oplus [X_{22} - X_{21}(\eta D + X_{11})^{-1}X_{12}].$$

Since $\mathrm{rank}\,([X_{21}\, X_{22}]) = \mathrm{rank}\,(X_{22})$, for sufficiently large $\eta > 0$ we have

$$X_{22} - X_{21}(\eta D/2)^{-1}X_{12} \in \mathrm{PSD}(n-r) \quad \text{and} \quad (\eta D/2)^{-1} - (\eta D + X_{11})^{-1} \in \mathrm{PD}_r.$$

Hence, under the positive semi-definite ordering $\succeq$, we have

$$X_{22} - X_{21}(\eta D + X_{11})^{-1}X_{12} \succeq X_{22} - X_{21}(\eta D/2)^{-1}X_{12} \succeq 0_{n-r}.$$

Thus, letting $P = X/\eta$ for sufficiently large η, we have $A + P = A + X/\eta \in \text{PSD}(n)$.

□

Remark 2.19 The proof of Proposition 2.18 is basically a Schur complement argument. We give the details for the sake of completeness.

Remark 2.20 Note that in Proposition 2.18 one needs only find an orthogonal matrix V such that $V^tAV = D \oplus 0$ for a positive definite matrix D, i.e., the last $n-r$ columns of V form an orthonormal basis for the kernel of A. The statement and the proof of the result will still be valid.

By Proposition 2.18, the zero matrix is the only element P in $\mathcal{S}$ such that $A + P \in \text{PSD}(n)$ if and only if the zero matrix is the only element X in $\mathcal{S}$ such that $V^tXV = (X_{ij})_{1\le i,j\le 2}$ with $X_{22} \in \text{PSD}(n-r)$ and $\text{rank}\,(X_{22}) = \text{rank}\,([X_{21}\ \ X_{22}])$. This condition can be checked by the following algorithm.

An algorithm Let $\mathcal{S}$ be a subspace of S_n, and $A \in \text{PSD}(n)$. Let V be an orthogonal matrix as described in Proposition 2.18.

Step 1 Construct a basis $\{X_1, \ldots, X_k\}$ for $\mathcal{S}$.

Step 2 Determine the dimension l of the space

$$\tilde{\mathcal{S}} = \left\{ [X_{21}\quad X_{22}] : V^tXV = \begin{pmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{pmatrix} \text{ with } X \in \mathcal{S} \right\}.$$

If $k > l$, then there is a nonzero $P \in \mathcal{S}$ such that $V^tPV = P_1 \oplus 0_{n-r}$ and $A + P \in$ PSD(n). Otherwise, go to Step 3.

Step 3 Determine whether there are real numbers $a_0, a_1, \ldots, a_k$ such that

$$Q = a_0A + a_1X_1 + \cdots + a_kX_k \in \text{PSD}(n)$$

with $(0_r \oplus I_{n-r}, V^tQV) = 1$.

If such a matrix Q exists, then there is a nonzero $P \in \mathcal{S}$ such that $A + P \in$ PSD(n). Otherwise, we can conclude that 0_n is the only matrix P in $\mathcal{S}$ such that $A + P \in \text{PSD}(n)$.

(Note that numerically Step 3 can be performed by existing software such as semi-definite programming routines, see [51] and [52].)

Explanation of the algorithm

Note that in Step 2, the condition $k > l$ holds if and only if there is a nonzero matrix $P \in \mathcal{S}$ such that $V^tPV = P_1 \oplus 0_{n-r}$ and $A + P \in \text{PSD}(n)$. To see this, let $V = [V_1|V_2]$ such that V_1 is $n \times r$. Then

$$\tilde{\mathcal{S}} = \{V_2^tXV : X \in \mathcal{S}\}$$

and $\{V_2^tX_1V, \ldots, V_2^tX_kV\}$ is a spanning set of $\tilde{\mathcal{S}}$. Clearly, $k \geq l$ and also, we can use this fact to find l. Transforming these matrices into vectors, l is the rank of the matrix with these vectors as columns.

If $k > l$, then there is a nonzero real vector $(a_1, \ldots, a_k)$ such that $a_1V_2^tX_1V + \cdots + a_kV_2^tX_kV = 0_{n-r,n}$. Since $X_1, \ldots, X_k$ are linearly independent, $X = a_1X_1 + \cdots + a_kX_k$

is nonzero. Therefore, V^tXV has the form $X_1 \oplus O_{n-r}$. By Proposition 2.18, there is $\delta > 0$ such that $A + \delta X \in \mathrm{PSD}(n)$.

Conversely, if there is a nonzero matrix $P \in \mathcal{S}$ such that $V^tPV = P_1 \oplus 0_{n-r}$ and $A + P \in \mathrm{PSD}(n)$, then there is a nonzero real vector $(a_1, \ldots, a_k)$ such that $P = a_1X_1 + \cdots + a_kX_k$ so that $a_1V_2^tX_1V + \cdots + a_kV_2^tX_kV = 0_{n-r,n}$. Hence, $\tilde{\mathcal{S}}$ has dimension less than k.

So, if $k = l$, and if there is a nonzero $P \in \mathcal{S}$ such that $A + P \in \mathrm{PSD}(n)$, then V_2^tPV cannot be zero. By Proposition 2.18, $V_2^tPV_2$ is nonzero, and Step 3 will detect such a matrix P if it exists.

By Proposition 2.18 and its proof, we have the following corollary.

Corollary 2.21 *Suppose* $\mathcal{S} \subseteq \mathbf{S}_n$, $A \in \mathrm{PSD}(n)$, *and the orthogonal matrix* V *satisfy the hypotheses of Proposition* 2.18.

(a) *If* $A \in \mathrm{PD}_n$, *then for any* $X \in \mathcal{S}$ *and sufficiently small* $\delta > 0$, *we have* $A+\delta X \in \mathrm{PD}_n$.

(b) *If there is an* $X \in \mathcal{S}$ *such that the matrix* X_{22} *in* (2.3.23) *is positive definite, then* $A + \delta X \in \mathrm{PD}_n$ *for sufficiently small* $\delta > 0$.

Remark 2.22 To use condition (b) in Corollary 2.21, one can focus on the matrix space

$$\mathcal{T} = \{V_2^tXV_2 : X \in \mathcal{S}\} \in \mathbf{S}_{n-r},$$

where V_2 is obtained from V by removing its first r columns. Note that PD_m is the interior of $\mathrm{PSD}(m)$, and

$$\mathrm{PSD}(m) = \{X \in \mathrm{S}_m : (X, P) \geq 0 \text{ for all } X \in \mathrm{PSD}(m)\}.$$

By the theorem of alternative (e.g., see [16]), $\mathcal{T} \cap \mathrm{PD}_{n-r} \neq \emptyset$ if and only if

$$\mathcal{T}^{\perp} \cap \mathrm{PSD}(n-r) = 0. \tag{2.3.25}$$

One can use standard semi-definite programming routines to check condition (2.3.25).

Here is another consequence of Proposition 2.18.

Corollary 2.23 *Suppose $\mathcal{S} \subseteq \mathrm{S}_n$, $A \in \mathrm{PSD}(n)$,* rank $(A) = n-1$ *and the orthogonal matrix V satisfy the hypotheses of Proposition* 2.18. *If $\mathcal{S}$ has dimension larger than $n-1$, then there is $X \in \mathcal{S}$ such that $A+\delta X \in \mathrm{PSD}(n)$ for all sufficiently small $\delta > 0$.*

Proof. If there is $X \in \mathcal{S}$ such that VXV^t has nonzero (n, n) entry, we may assume that it is positive; otherwise replace X by $-X$. Then by Proposition 2.18 $A + \delta X \in \mathrm{PSD}(n)$ for sufficiently small $\delta > 0$. Suppose VXV^t always has zero entry at the (n, n) position. Since $\mathcal{S}$ has dimension at least n, there exists a nonzero $X \in \mathcal{S}$ such that the last column of VXV^t are zero. So, $A + \delta X \in \mathrm{PSD}(n)$ for sufficiently small $\delta > 0$. □

2.3.3 Application of results

Next, we can use Proposition 2.18 to answer the question raised in [1].

Proposition 2.24 *Let $\mathbf{S}_n^0$ be the subspace of matrices in $\mathbf{S}_n$ with all diagonal entries equal to zero. Let $A \in \mathcal{D}(n)$, and $\mathcal{S}$ be a subspace of $\mathbf{S}_n^0$. Suppose U is $n \times (n-1)$ such that $U^t e = 0$, $U^t U = I_{n-1}$, and $-U^t A U = \operatorname{diag}(d_1, \ldots, d_r, 0, \ldots, 0)$, where $d_1 \geq \cdots \geq d_r > 0$. Then there is a nonzero matrix $P \in \mathcal{S}$ such that $A + P \in \mathcal{D}(n)$ if and only if there is nonzero matrix $X \in \mathcal{S}$ such that*

$$U^t X U = \begin{pmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{pmatrix} \tag{2.3.26}$$

with $X_{22} \in \mathrm{PSD}(n-1-r)$ and $\operatorname{rank}(X_{22}) = \operatorname{rank}([X_{21}\ X_{22}])$.

Proof. By the result in [12], the mapping $X \mapsto -\frac{1}{2}U^t X U$ is a linear isomorphism from $\mathbf{S}_n^0$ to $\mathbf{S}_{n-1}$ such that the cone $\mathcal{D}(n)$ is mapped onto $\mathrm{PSD}(n-1)$. Thus, the existence of a nonzero $X \in \mathcal{S}$ such that $A + X \in \mathcal{D}(n)$ is equivalent to the existence of a nonzero $Y \in \{-\frac{1}{2}U^t X U : X \in \mathcal{S}\}$ such that $-\frac{1}{2}A + Y \in \mathrm{PSD}(n-1)$. One can therefore apply Proposition 2.18 to get the conclusion. □

Accordingly, we have the following corollary concerning unique ESD matrix completion. Part (a) in the following was also observed in [1, Theorem 3.1].

Corollary 2.25 *Use the notations in Proposition* 2.24.

(a) *If $U^t A U$ has rank $n-1$, then for any $X \in \mathcal{S}$ and sufficiently small $\delta > 0$, we have $A + \delta X \in \mathcal{D}(n)$*

(b) *If there is an $X \in \mathcal{S}$ such that the matrix X_{22} in* (2.3.26) *is positive definite, then $A + \delta X \in \mathcal{D}(n)$ for sufficiently small $\delta > 0$.*

(c) *If* rank $(U^t A U) = n-2$ *and* $\mathcal{S}$ *has dimension larger than* $n-2$, *then there is an* $X \in \mathcal{S}$ *such that* $A + \delta X \in \mathcal{D}(n)$ *for all sufficiently small* $\delta > 0$.

Note that Proposition 2.18 is also valid for the real space $\mathbf{H}_n$ of $n \times n$ complex Hermitian matrices. Moreover, our techniques can be applied to other completion problems on the space $\mathbf{M}_{m,n}$ of $m \times n$ complex matrices that can be formulated in terms of positive semi-definite matrices. For instance, for any $B \in \mathbf{M}_{m,n}$, the operator norm $\|B\| \leq 1$ if and only if

$$\begin{pmatrix} I_m & B \\ B^* & I_n \end{pmatrix} \in \mathrm{PSD}(m+n).$$

As a result, if $\tilde{\mathcal{S}}$ is a subspace of $\mathbf{M}_{m,n}$, and $\tilde{A} \in \mathbf{M}_{m,n}$ such that $\|\tilde{A}\| \leq 1$, we can let

$$A = \begin{pmatrix} I_m & \tilde{A} \\ \tilde{A}^* & I_n \end{pmatrix} \in \mathrm{PSD}(m+n),$$

and $\mathcal{S}$ be the subspace of $\mathbf{H}_{m+n}$ consisting of matrices of the form

$$X = \begin{pmatrix} 0_m & \tilde{X} \\ \tilde{X}^* & 0_n \end{pmatrix}$$

with $\tilde{X} \in \tilde{\mathcal{S}}$. Then there is $\tilde{X} \in \tilde{\mathcal{S}}$ such that $\|\tilde{A} + \tilde{X}\| \leq 1$ if and only if there is $X \in \mathcal{S}$ such that $A + X \in \mathrm{PSD}(m+n)$. We can then apply Proposition 2.18 to determine the uniqueness condition.

2.3.4 Examples and additional remarks

We illustrate how to use our results and algorithm in the previous section in the following. We begin with the positive semi-definite matrix completion problem in the general setting.

Example 2.26 Let

$$A_1 = I_6 \oplus [0], \quad A_2 = I_5 \oplus 0_2, \quad A_3 = I_4 \oplus 0_3 \quad \text{and} \quad A_4 = I_3 \oplus 0_4.$$

Let $b = 1/\sqrt{2}$ and $\mathcal{S} = \operatorname{span}\{X_1, X_2, X_3, X_4\}$ where

$$X_1 = \begin{bmatrix} -1 & 0 & -1 & 0 & -1 & -b & b \\ 0 & 1 & 0 & 1 & 0 & b & b \\ -1 & 0 & -1 & 0 & -1 & -b & b \\ 0 & 1 & 0 & 1 & 0 & b & b \\ -1 & 0 & -1 & 0 & -1 & -b & b \\ -b & b & -b & b & -b & 0 & 1 \\ b & b & b & b & b & 1 & 0 \end{bmatrix}, \quad X_2 = \begin{bmatrix} -1 & -1 & 0 & 0 & -1 & -b & -b \\ -1 & -1 & 0 & 0 & -1 & -b & -b \\ 0 & 0 & 1 & 1 & 0 & b & -b \\ 0 & 0 & 1 & 1 & 0 & b & -b \\ -1 & -1 & 0 & 0 & -1 & -b & -b \\ -b & -b & b & b & -b & 0 & -1 \\ -b & -b & -b & -b & -b & -1 & 0 \end{bmatrix}$$

$$X_3 = \begin{bmatrix} -1 & 1 & 0 & 0 & -1 & b & b \\ 1 & -1 & 0 & 0 & 1 & -b & -b \\ 0 & 0 & 1 & -1 & 0 & b & -b \\ 0 & 0 & -1 & 1 & 0 & -b & b \\ -1 & 1 & 0 & 0 & -1 & b & b \\ b & -b & b & -b & b & 0 & -1 \\ b & -b & -b & b & b & -1 & 0 \end{bmatrix},$$

$$X_4 = \begin{bmatrix} -1 & 0 & 1 & 0 & -1 & b & -b \\ 0 & 1 & 0 & -1 & 0 & b & b \\ 1 & 0 & -1 & 0 & 1 & -b & b \\ 0 & -1 & 0 & 1 & 0 & -b & -b \\ -1 & 0 & 1 & 0 & -1 & b & -b \\ b & b & -b & -b & b & 0 & 1 \\ -b & b & b & -b & -b & 1 & 0 \end{bmatrix}.$$

Then for A_1, A_2, A_3, there exists a nonzero $P \in \mathcal{S}$ such that $A_i + \delta P \in \text{PSD}(7)$ for sufficiently small $\delta > 0$. For A_4, the zero matrix is the unique element X in $\mathcal{S}$ such that $A_4 + X$ is positive semi-definite.

To see the above conclusion, we use the algorithm in the last section. Clearly, we can let $V = I_7$ be the orthogonal matrix in the algorithm.

Suppose $A = A_1$. Applying Step 2 of the algorithm with $V_2 = e_7$, we see that $k = \dim \mathcal{S} = 4 > 2 = \dim\{V_2^t X_j : j = 1, 2, 3, 4\}$. So, there is non-zero $X \in \mathcal{S}$ such that $A + \delta P \in \text{PSD}(7)$ for sufficiently small $\delta > 0$. In fact, if P is a linear combination of $X_1 + X_2$ and $X_3 + X_4$, then for sufficiently small $\delta > 0$, $A + \delta P \in \text{PSD}(7)$.

Suppose $A = A_2$. Applying Step 2 of the algorithm with $V_2 = [e_6 \,|\, e_7]$, we see that $k = \dim \mathcal{S} = 4 > 3 = \dim\{V_2^t X_j : j = 1, 2, 3, 4\}$. So, there is non-zero $X \in \mathcal{S}$ such that $A + \delta P \in \text{PSD}(7)$ for sufficiently small $\delta > 0$. In fact, this is true for

$\delta \in [-1/4, 1/8]$ and

$$P = \sum_{i=1}^{4} X_i = \begin{bmatrix} -4 & 0 & 0 & 0 & -4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4 & 0 & 0 & 0 \\ -4 & 0 & 0 & 0 & -4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}. \tag{2.3.27}$$

Suppose $A = A_3$. Applying Step 2 of the algorithm with $V_2 = [e_5 \,|\, e_6 \,|\, e_7]$, we see that $k = l = 4$; we proceed to step 3. If P is defined as in (2.3.27), $Q = \alpha A - \frac{1}{4}P \in \text{PSD}(7)$ where $\alpha \geq 1$. Thus, we get the desired conclusion on A_3.

Note that one can also use standard semi-definite programming packages to draw our conclusion in Step 3. To do that we consider the following optimization problem:

$$\text{Minimize (or Maximize) } (C, Q) \text{ subject to } (B_i, Q) = b_i \text{ and } Q \in \text{PSD}(n).$$

Since we are interested only in feasibility, we can set C to be the zero matrix. To ensure that $Q = a_0 A + a_1 X_1 + \cdots + a_4 X_4 \in \text{PSD}(n)$, we set the matrices $\{B_i\}$, for $i = 1, \ldots, m$, to be a basis of $(\mathcal{S} \cup \{A\})^{\perp}$ in $\mathbf{S}_7$ and set $b_i = 0$. Then set $B_{m+1} = 0_4 \oplus I_3$ with $b_{m+1} = 1$. We will get the desired conclusion by running any standard semi-definite programming package.

Suppose $A = A_4 \in \text{PSD}(7)$. Applying Step 2 of the algorithm with $V_2 = [e_4 \,|\, e_5 \,|\, e_6 \,|\, e_7]$, we see that $k = l = 4$; we proceed to step 3. Since I_4 is orthogonal to all matrices in $\tilde{S} = \operatorname{span}\{V_2^t X_j V_2 : j = 1, \ldots, 4\}$, we see that $I_4 \in \tilde{S}^{\perp} \cap \mathrm{PD}_4$. By the theorem of alternative, $\tilde{S} \cap \mathrm{PSD}(4) = \{0_4\}$. Thus, there is no matrix Q satisfying Step 3, and 0_7 is the only element X in S such that $A_4 + X \in \mathrm{PSD}(7)$.

Actually, to get the conclusion on A_4 one can also check directly that the matrix Q in Step 3 of the algorithm does not exist by a straightforward verification or using standard semi-definite programming routines.

We can use Example 2.26 to get examples for the ESD matrix completion problem in the following. Denote by $\{E_{11}, E_{12}, \ldots, E_{nn}\}$ the standard basis for $n \times n$ real matrices.

Example 2.27 Let $A_1, A_2, A_3, A_4, X_1, X_2, X_3, X_4$ be defined as in Example 2.26. Suppose $\tilde{A}_1, \tilde{A}_2, \tilde{A}_3, \tilde{A}_4 \in \mathcal{D}(8)$ are such that

$$\frac{-1}{2} U^t \tilde{A}_j U = A_j, \qquad j = 1, 2, 3, 4,$$

where

$$U = \frac{1}{\sqrt{8}} \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & \sqrt{2} & 0 \\ 1 & -1 & -1 & 1 & 1 & -\sqrt{2} & 0 \\ -1 & 1 & -1 & 1 & -1 & 0 & \sqrt{2} \\ -1 & -1 & 1 & 1 & -1 & 0 & -\sqrt{2} \\ 1 & 1 & 1 & -1 & -1 & -\sqrt{2} & 0 \\ 1 & -1 & -1 & -1 & -1 & \sqrt{2} & 0 \\ -1 & 1 & -1 & -1 & 1 & 0 & -\sqrt{2} \\ -1 & -1 & 1 & -1 & 1 & 0 & \sqrt{2} \end{bmatrix}.$$

Note that the matrices $\tilde{A}_1, \ldots, \tilde{A}_4$ are determined uniquely by the result in [12]. Let $\mathcal{S} = \text{span}\{E_{13}+E_{31}, E_{14}+E_{41}, E_{23}+E_{32}, E_{24}+E_{42}\}$. Then

$$\frac{-1}{2}U^t(E_{13}+E_{31})U = \frac{-1}{8}X_1, \quad \frac{-1}{2}U^t(E_{14}+E_{41})U = \frac{-1}{8}X_2,$$

$$\frac{-1}{2}U^t(E_{23}+E_{32})U = \frac{-1}{8}X_3, \quad \frac{-1}{2}U^t(E_{24}+E_{42})U = \frac{-1}{8}X_4.$$

By Proposition 2.24 and Example 2.26, we see that there exists a nonzero $P \in \mathcal{S}$ such that $\tilde{A}_j + P \in \mathcal{D}(8)$ for $j = 1, 2, 3$, and 0_8 is the unique element X in $\mathcal{S}$ such that $\tilde{A}_4 + X \in \mathcal{D}(8)$.

In fact, we can present Example 2.27 in the standard completion problem setting. For instance, suppose A_0 is the partially specified matrix

$$A_0 = \begin{bmatrix} 0 & 2 & ? & ? & 2 & 2 & 7/4 & 7/4 \\ 2 & 0 & ? & ? & 2 & 2 & 7/4 & 7/4 \\ ? & ? & 0 & 1 & 7/4 & 7/4 & 1 & 2 \\ ? & ? & 1 & 0 & 7/4 & 7/4 & 2 & 1 \\ 2 & 2 & 7/4 & 7/4 & 0 & 2 & 7/4 & 7/4 \\ 2 & 2 & 7/4 & 7/4 & 2 & 0 & 7/4 & 7/4 \\ 7/4 & 7/4 & 1 & 2 & 7/4 & 7/4 & 0 & 1 \\ 7/4 & 7/4 & 2 & 1 & 7/4 & 7/4 & 1 & 0 \end{bmatrix}.$$

We can complete A_0 to $\tilde{A}_1$ by setting all unspecified entries to 7/4. So, we have $\frac{-1}{2}U^t\tilde{A}_1U = A_1$. If P is a linear combination of $E_{13}+E_{31}+E_{14}+E_{41}$ and $E_{23}+E_{32}+E_{24}+E_{42}$, then $\tilde{A}_1 + \delta P \in \mathcal{D}(8)$ for sufficiently small $\delta > 0$.

Remark 2.28 Continue to use the notations in Example 2.27, and let $Y \in \mathbf{S}_8^0$ be such that $-U^tYU/2 = 0_6 \oplus [1]$. We have $(U^tYU, U^tXU) = 0$ for any $X \in \mathcal{S}$. Then [1, Theorem 3.3 (2.a)] asserts that there exists a unique completion A_0, which is not true by Example 2.27. Likewise, if $Y \in \mathbf{S}_8^0$ is such that $-U^tYU/2 = 0_5 \oplus I_2$, then the partial matrix corresponding to $\tilde{A}_2$ has more than one ESD matrix completion, which disagrees with [1, Theorem 3.3 (2.b)].

The flaw in [1, Theorem 3.3] lies in the proof of Theorem 3.2 (Corollary 4.1) in the paper. Let

$$\mathcal{L} = \{-U^tXU/2 : X \in \mathcal{S}\}, \quad \mathcal{L}^\perp = \{X \in \mathbf{S}_{n-1} : (X, Z) = 0 \text{ for all } Z \in \mathcal{L}\},$$

$$K = \{B \in \mathbf{S}_{n-1} : B = \lambda(X + \frac{1}{2}U^tA_0U), \lambda \geq 0, X \in \mathrm{PSD}(n-1)\}$$

and

$$\mathrm{int}(K^\circ) = \{C \in \mathbf{S}_{n-1} : (C, B) < 0 \text{ for all } B \in K\}.$$

The author of [1] claimed that: *if there exists some* $Y \in \mathrm{PD}_{n-1-r}$ *such that*

$$\hat{Y} = \begin{pmatrix} 0 & 0 \\ 0 & Y \end{pmatrix} \in \mathcal{L}^\perp, \tag{2.3.28}$$

then

$$\mathcal{L}^\perp \cap \mathrm{int}(K^\circ) \neq \emptyset, \tag{2.3.29}$$

and hence $\mathcal{L} \cap \mathrm{cl}(K) = \{0\}$ by the theorem of alternative. However, in Example 2.27, in spite of the existence of $\hat{Y} \in \mathcal{L}^\perp$ of the form (2.3.28) one can check that (2.3.29) does not hold. In particular, $\hat{Y} \notin \mathrm{int}(K^\circ)$ because $I_r \oplus 0_{n-1-r} \in K$ but $(\hat{Y}, I_r \oplus 0_{n-1-r}) = 0$.

2.4 Spherical ESD Matrices

In this section, we are interested in a subset of $\mathcal{D}$, the Euclidean squared distance (ESD) matrices, which we call spherical ESD matrices. They are those $A \in \mathcal{D}$ that admit a configuration of points that not only have centroid at the origin but also all lie on a sphere whose center is the origin. Such points are commonly called regular figures, see [22].

Distance matrices are of interest in molecular biology and structural chemistry. They are used to determine structure of molecules based only on information about the distances between atoms. There has been recent interest in trying to determine molecular structure from incomplete and error-filled data. One approach is to look at substructures within a molecule that display certain properties and use those substructures to help determine the full structure of the molecule. One simple and common structure is that of a regular figure and the corresponding distance matrix is a spherical ESD matrix.

We let $\hat{\mathcal{D}}(n)$ be the subset of $\mathcal{D}(n)$ whose matrices A admit a configuration of points $x_1, \ldots, x_n$ which lie on a sphere whose center is the centroid of the points. In other words, if $A \in \hat{\mathcal{D}}(n)$ then $A = ||x_i - x_j||^2$ where $\sum_{i=1}^n x_i = 0$ and there is some a such that $||x_i||^2 = a$ for all $i = 1, \ldots, n$. Formally, we define

$$\hat{\mathcal{D}}(n) = \{A \in \mathcal{D}(n) : Ae = \lambda e\}.$$

It is not immediately obvious that the set just defined is the same as the set described above. In the next subsection, We characterize spherical ESD matrices and see that these two descriptions are indeed the same. We also discuss why a characterization theorem as in the first section is not practical. We will review some known results, see [22], and mention a few new ones. In particular, we will discuss some of the geometry of the cone of these matrices and the forms of the linear preservers of the span of this set.

2.4.1 Characterizations

We have defined the linear mappings $\tau : \mathbf{S}_n \to \mathbf{S}_n$ and $\kappa : \mathbf{S}_n \to \mathbf{S}_n$ by

$$\tau(A) = -\frac{1}{2}(I - \frac{1}{n}J)A(I - \frac{1}{n}J) \tag{2.4.30}$$

and

$$\kappa(B) = D_B J + J D_B - 2B \tag{2.4.31}$$

where D_B are just the diagonal entries of B. Note that throughout this section, we are considering the instance where $w = e$. We begin by presenting a characterization theorem similar to the one in the first section of this chapter. It is, however, significantly shorter, as the majority of the characterizations of ESD matrices become far too impractical and cumbersome.

Theorem 2.29 *Suppose A is an $n \times n$ predistance matrix. Let U be any $n \times (n-1)$ matrix for which the $n \times n$ matrix $V = [\frac{e}{n}|U]$ is orthogonal. Then the following are equivalent.*

(a) *$Ae = \lambda e$ and there exists an e-centered spanning set of $\mathbf{R}^k$, $\{x_1, \ldots, x_n\}$ for which $A = \|x_i - x_j\|^2$.*

(b) *There exists an e-centered spanning set of* $\mathbf{R}^k$, $\{x_1, \ldots, x_n\}$ *and an* $a > 0$ *for which* $\tau(A) = (x_i^t x_j)$ *and such that* $(\tau(A))_{ii} = \|x_i\|^2 = a$ *for all* i.

(c) *The matrix*

$$V^t A V = \begin{bmatrix} 2na & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & U^t A U & \\ 0 & & & \end{bmatrix}$$

where $U^t A U$ *is negative semidefinite of rank* k *such that the diagonal entries of* $UU^t AUU^t$ *all equal* $-2a$.

Proof.

(a) ⇔ (b) Because of Theorem 2.1, we need only show that $Ae = \lambda e$ if and only if there exists some $a > 0$ such that $(\tau(A))_{ii} = a$ for all i. Condition (c) of Theorem 2.1 and trace $(A) = 0$ suffices to show that $\lambda > 0$ if such a λ exists. Recall that $\kappa \circ \tau(A) = A$ as $A \in \mathcal{D}(n)$. Letting $B = \tau(A)$ and D_B the diagonal matrix $I_n \circ B$, we see that

$$A = \kappa(B) = D_B J + J D_B - 2B.$$

Because $Be = 0$ and $JD_B e = (\text{trace}\,(B))e$, it follows that $Ae = \lambda e$ if and only if $D_B e = \frac{1}{n}(\lambda - \text{trace}\,(B))e$. But this occurs if and only if the diagonals B all have the same value, i.e. $(B)_{ii} = a = \frac{1}{n}(\lambda - \text{trace}\,(B))$ for all i. This also shows that $\lambda = 2na$.

(a) $\Rightarrow$ (c) Because $Ae = \lambda e$, $V^tAV = [\lambda] \oplus U^tAU$. Furthermore, U^tAU is negative semidefinite of rank k by Theorem 2.1. Since (a) and (b) are equivalent and $UU^tAUU^t = -2\tau(A)$, the diagonals of UU^tAUU^t are $-2(\tau(A))_{ii} = -2a$ where $\lambda = 2na$.

(c) $\Rightarrow$ (b) Suppose the matrix

$$V^tAV = \begin{bmatrix} 2na & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & U^tAU & \\ 0 & & & \end{bmatrix}$$

where U^tAU is negative semidefinite of rank k such that the diagonal entries of UU^tAUU^t all equal $-2a$. By Theorem 2.1, there exists an e-centered spanning set of $\mathbf{R}^k$, $\{x_1, \ldots, x_n\}$ for which $\tau(A) = (x_i^t x_j)$. Note that $UU^tAUU^t = -2\tau(A)$. Hence $(\tau(A))_{ii} = a$ for some $a > 0$. □

The equivalence of (a) and (b) was previously shown in [22]. Note that our description of $\hat{\mathcal{D}}(n)$ is evident in our statement (b). We use the origin as the center of the sphere ($\|x_i\|^2 = a$ for all i) and as the centroid of the points ($x_1, \ldots, x_n$ are e–centered). Considering this set of matrices formed by transforming the matrices in $\hat{\mathcal{D}}(n)$, we get the subset $\hat{\mathcal{G}}(n) \subset \mathrm{PSD}(n)$ consisting of matrices A such that $Ae = 0$ and the diagonal entries of A are constant. Equivalently, $\hat{\mathcal{G}}(n)$ consists of positive scalar multiples of the subset of the $n \times n$ correlation matrices $C \in \mathcal{E}$ such that $Ce = 0$. While condition (c) was not shown in their paper, it is because it is not a convenient characterization. One could replace condition (c) with a simpler statement involving only the U^tAU part, but the inclusion of the column $e/\sqrt{n}$ to make the matrix V lets us state the following as a obvious corollary. For more on the Perron-Frobenius theorem, see [25, pp. 500,508]

Corollary 2.30 *If $A \in \hat{\mathcal{D}}(n)$ then e is the Perron vector with eigenvalue $2na$ where a is the radius of the sphere the points lie on.*

This theorem also tells us more about the mapping τ and κ. Recall that by restricting the domains to $[\mathcal{D}(n)]$ and $[\mathcal{G}(n)]$, the mappings $\tau : [\mathcal{D}(n)] \to [\mathcal{G}(n)]$ and $\kappa : [\mathcal{G}(n)] \to [\mathcal{D}(n)]$ as defined in 2.4.30 and 2.4.31 are invertible. We see that by further restricting the domains to $[\hat{\mathcal{D}}(n)]$ and $[\hat{\mathcal{G}}(n)]$, the mappings $\tau : [\hat{\mathcal{D}}(n)] \to [\hat{\mathcal{G}}(n)]$ and $\kappa : [\hat{\mathcal{G}}(n)] \to [\hat{\mathcal{D}}(n)]$ are also invertible. In fact, when we so restrict τ and κ, these mappings will have the following forms.

$$\tau(A) = -\frac{1}{2}A + aJ \tag{2.4.32}$$

and

$$\kappa(B) = 2bJ - 2B \tag{2.4.33}$$

where a is the square of the radius of the sphere and b are the diagonal entries of B. We can use this knowledge to determine the forms of linear preservers of $\hat{\mathcal{D}}(n)$ by looking at linear preservers of $\hat{\mathcal{G}}(n)$. We do this in the next section.

2.4.2 Linear preservers of $\hat{\mathcal{D}}(n)$

To further examine the set $\hat{\mathcal{D}}(n)$, it is necessary to use the transformation τ and the resulting relationship between $\hat{\mathcal{D}}(n)$ and $\hat{\mathcal{G}}(n)$. When dealing with $\mathcal{D}(n)$, we instead used the transformation from $\mathcal{D}(n)$ to PSD$(n-1)$. The added condition that the points all lie on a sphere adds a complexity such that looking at an appropriate subset of PSD$(n-1)$ is too unwieldy to help, see condition (c) of Theorem 2.29.

In section 2.2, two of the three results on $\mathcal{D}(n)$ focused on the embedding dimension of the matrices. This corresponds to the rank of the matrices in $\mathcal{G}(n)$. Define

$$\hat{\mathcal{G}}_k(n) = \{A \in \hat{\mathcal{G}}(n) : \text{rank}(A) = k\}.$$

Note that the notation $\hat{\mathcal{G}}_k$ will replace $\hat{\mathcal{G}}_k(n)$ when it is clear from the context what size matrices are being considered. It is not hard to see that for n odd, $\hat{\mathcal{G}}_1(n)$ is the empty set and for n even, it is the positive multiples of a finite set of matrices. Thus, for different values of n, different results can be shown. We focus on the the particular problem of finding the form of the linear maps $\psi : [\hat{\mathcal{D}}(n)] \to [\hat{\mathcal{D}}(n)]$ such that $\psi(\hat{\mathcal{D}}(n)) = \hat{\mathcal{D}}(n)$. We first solve the corresponding problem of finding the form of the linear maps $\phi : [\hat{\mathcal{G}}(n)] \to [\hat{\mathcal{G}}(n)]$ such that $\phi(\hat{\mathcal{G}}(n)) = \hat{\mathcal{G}}(n)$. For the even case, this problem is not too hard to solve, though the details take quite a bit to get through. For the odd case, this problem remains unsolved. Throughout the rest of this section, we will assume that n is even, unless explicitly stated otherwise.

We first need to look at some geometric properties of $\hat{\mathcal{G}}(n)$. For all $A \in \hat{\mathcal{G}}_k(n)$, we can find a matrix $V = [v_1 ... v_n] \in M_{k,n}(\mathbf{R})$ such that $A = V^t V$. Note that since the diagonal entries of A are all equal, this means that for all i, j, $v_i^t v_i = v_j^t v_j$. This V is not unique and, in fact, can be replaced by QV where Q is any $k \times k$ orthogonal matrix.

The $n \times n$ matrix X is a perturbation of $A \in \hat{\mathcal{G}}(n)$, written $X \in \mathcal{P}_A$, if and only if there is some $\delta > 0$ such that $A \pm \epsilon X \in \hat{\mathcal{G}}(n)$ for all $0 < \epsilon < \delta$. If $A = V^t V \in \hat{\mathcal{G}}(n)$, then the set of perturbations of A, $\mathcal{P}_A$ is

$$\mathcal{P}_A = \{V^t R V : R = R^t \in M_k(\mathbf{R}), v_i^t R v_i = v_1^t R v_1 \text{ for all } i\}.$$

The property that $R = R^t$ ensures symmetry of the perturbation and $v_i^t R v_i = v_1^t R v_1$ is needed so that diagonal entries all agree. Note that if $X = \gamma A$ for some γ, then clearly $X \in \mathcal{P}_A$. We can see that $\mathcal{P}_A$ can be divided up into two parts, namely, $\mathcal{P}_A = \langle A \rangle \oplus \mathcal{P}_{A^\perp}$ where $\mathcal{P}_{A^\perp} = \mathcal{P}_A \bigcap A^\perp$. In other words, if $X \in \mathcal{P}_A$, then $X = \lambda A + (X - \lambda A)$ where $\lambda = \operatorname{tr} X / \operatorname{tr} A$. The matrix $X - \lambda A \in \mathcal{P}_{A^\perp}$, and $\operatorname{tr}(X - \lambda A) = 0$.

Let $A = V^t V \in \hat{\mathcal{G}}(n)$, with $V = [v_1 ... v_n]$, $v_i \in \mathbf{R}^r$ where $r = \operatorname{rank}(A)$ and $t_A = \dim(\operatorname{span}\{v_1 v_1^t, ..., v_n v_n^t\})$. Then

$$\dim \mathcal{P}_A = \frac{r(r+1)}{2} + 1 - t_A.$$

The number of free entries in $R = R^t$ gives the $\frac{r(r+1)}{2}$ term. The $+1$ term reflects that we can add multiples of A and the $-t_A$ term describes the number of constraints imposed by assuming $v_i^t R v_i = v_1^t R v_1$ for all i. This condition is equivalent to $\operatorname{trace}(v_i^t R v_i) = \operatorname{trace}(v_1^t R v_1)$, which implies $\operatorname{trace}(v_i v_i^t R) = \operatorname{trace}(v_1 v_1^t R)$. Thus we are interested in the number of linearly independent matrices of the form $v_i v_i^t$. Note that $r \leq t_A \leq \max\{n, r(r+1)/2\}$.

Before we proceed, we prove the following fact.

Lemma 2.31 *Suppose* $A \in \hat{\mathcal{G}}(n)$ *and* P *is an* $n \times n$ *permutation matrix. Then* $P^t \mathcal{P}_A P = \mathcal{P}_{P^tAP}$.

Proof. Suppose $A \in \hat{\mathcal{G}}(n)$ and P is an $n \times n$ permutation matrix. Then $X \in P^t \mathcal{P}_A P$ if and only if $PXP^t \in \mathcal{P}_A$. But $PXP^t \in \mathcal{P}_A$ if and only if there exists a δ such that $A + \epsilon PXP^t \in \hat{\mathcal{G}}(n)$. By our supposition, this occurs if and only if $P^tAP + \epsilon X \in \hat{\mathcal{G}}(n)$ which is equivalent to saying $X \in \mathcal{P}_{P^tAP}$. □

We can divide $\hat{\mathcal{G}}(n)$ into the following subsets which will be useful later. Let

$$\mathcal{P}_k = \{A \in \hat{\mathcal{G}}(n) : \dim \mathcal{P}_A = k\}.$$

Since we are also interested in the rank of the matrices of $\hat{\mathcal{G}}(n)$, we also consider the following subsets. Let

$$\mathcal{C}_k = \{A \in \hat{\mathcal{G}}_k(n) : \dim\, \mathcal{P}_A = \frac{k(k+1)}{2} + 1 - k\}.$$

If $A \in \hat{\mathcal{G}}_1(n)$ then $\mathcal{P}_A$ will have dimension 1, therefore, $\mathcal{C}_1 = \hat{\mathcal{G}}_1(n)$. Following the proof of the following proposition, it can be seen that an alternative definition will be needed for n odd.

Proposition 2.32 *Suppose* $n = 2m$. *Then*

$$\mathcal{C}_k = \{A \in \hat{\mathcal{G}}(n) : A = V^tV \text{ where } V = V_0[I_k\ Q\ \ -I_k\ \ -Q]P\}$$

where $V_0 \in M_k(\mathbf{R})$ *is an invertible matrix with column vectors all the same Euclidean length,* $Q \in M_{k,m-k}(\mathbf{R})$ *such that each column of* Q *has exactly one nonzero entry which is equal to* 1 *and* P *is an* $n \times n$ *permutation matrix.*

Proof. By construction, if A is in the set described above, then $t_A = k$. Therefore, $\dim \mathcal{P}_A = \frac{k(k+1)}{2} + 1 - k$ and so $A \in \mathcal{C}_k$. Now, assume $A \in \mathcal{C}_k$. Since $A \in \hat{\mathcal{G}}_k(n)$, there exists a $W \in M_{n,k}(\mathbf{R})$ with rank $(W) = k$ such that $A = W^tW$. Since there are k independent columns in W, label them $w_{i_1}, ..., w_{i_k}$. Thus, $w_{i_1}w_{i_1}^t, ..., w_{i_k}w_{i_k}^t$ are also linearly independent. By the dimension of $\mathcal{P}_A$, there must be exactly k linearly independent $w_jw_j^t$, namely the ones listed. Therefore, for all $j \in \{i_{k+1}, ..., i_m\}$, there exists an $a_1, ..., a_k$ not all zero such that

$$w_jw_j^t = \sum_{l=1}^{k} a_l w_{i_l} w_{i_l}^t = \begin{pmatrix} w_{i_1} & \cdots & w_{i_k} \end{pmatrix} \begin{pmatrix} a_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & a_k \end{pmatrix} \begin{pmatrix} w_{i_1}^t \\ \vdots \\ w_{i_k}^t \end{pmatrix}.$$

Since $[w_{i_1} \cdots w_{i_k}]$ is $k \times k$ and full rank, and hence invertible, therefore, it preserves rank. Since $w_jw_j^t$ is rank one, there is only one value of $a_1, ..., a_k$ that is nonzero, call it a_l. Since the trace is also the same, $a_l = 1$, in other words, $w_jw_j^t = w_lw_l^t$ where $l \in \{i_1, ..., i_k\}$. Thus, for each $j \in \{i_{k+1}, ..., i_m\}$, there is an $l \in \{i_1, ..., i_k\}$ such that $w_j = \pm w_l$. Recall that $0 = W^te = \sum_{i=1}^{n} w_i$ and each $w_i \in \{\pm w_{i_1}, ..., \pm w_{i_k}\}$, therefore, $0 = n_1 w_{i_1} + ... + n_k w_{i_k}$. But since $w_{i_1}, ..., w_{i_k}$ are linearly independent, $n_1 = ... = n_k = 0$. Thus, for each $l \in \{i_1, ..., i_k\}$, w_l occurs the same number of times in W as does $-w_l$. Thus $W = V$ where V is described in the statement of the Proposition. □

This gives us the following corollary.

Corollary 2.33 *For n even and $k = \frac{r(r+1)}{2} + 1 - r = \frac{r(r-1)}{2} + 1$, let $A = V^tV \in \hat{\mathcal{G}}_r(n)$.*

Then $A \in \mathcal{P}_k$ (i.e. $t_A = r$) implies

$$(\#\text{ of times } v_i \text{ is a column of } V) = (\#\text{ of times } (-v_i) \text{ is a column of } V).$$

We now examine the relationship between $\mathcal{C}_k$ for different values of k.

Proposition 2.34 *Let $n = 2m$. Then $\overline{\mathcal{C}_k} = \bigcup_{j\leq k} \mathcal{C}_j$.*

Proof. Suppose X is in $\overline{\mathcal{C}_k}$. Either $X \in \mathcal{C}_k$, and we are done, or there exists a sequence of elements of $\mathcal{C}_k$ that converge to X. In other words $\{P(r)V^t(r)V(r)P^t(r)\} \rightarrow X$ where $V(r)$ is a $k \times k$ matrix such that

$$V(r) = [v_1(r) \ \cdots \ v_k(r)][I_k \ \ -I_k \ Q(r) \ \ -Q(r)],$$

where $Q(r)$ is a $k \times (m-k)$ $(0,1)$–matrix with exactly one nonzero entry in each column. Since there are a finite number of $n \times n$ permutation matrices, divide the sequence up by each type of permutation P. At least one such subsequence will converge; consider that subsequence. Since there are only a finite number of $(0,1)$–matrices of size $k \times (m-k)$, divide the sequence up by each type of matrix Q. Since there are only a finite number of subsequences, one must be convergent; choose that one. Thus we have a sequence $PV^t(r)V(r)P^t \rightarrow X$ where $V(r) = [v_1(r) \ \cdots \ v_k(r)][I_k \ \ -I_k \ Q \ \ -Q]$. Clearly, then X will be of the form $X = PW^tWP^t$ where

$$W = [w_1 \ \cdots \ w_k][I_k \ \ -I_k \ Q \ \ -Q].$$

Since $\{w_1, ..., w_k\}$ might not be linearly independent, this might not be in $\mathcal{C}_k$, but then, by Proposition 2.32, it will be in $\mathcal{C}_j$ where j is the number of linearly independent vectors in $\{w_1, ..., w_k\}$. □

We now consider linear mappings $\phi : [\hat{\mathcal{G}}(n)] \to [\hat{\mathcal{G}}(n)]$ such that $\phi(\hat{\mathcal{G}}(n)) = \hat{\mathcal{G}}(n)$. For n even we will show the forms of of such mappings and briefly discuss what happens when n is odd. First we show the following three lemmas.

Lemma 2.35 *Let $\phi : [\hat{\mathcal{G}}(n)] \to [\hat{\mathcal{G}}(n)]$ be a linear mapping such that $\phi(\hat{\mathcal{G}}(n)) = \hat{\mathcal{G}}(n)$ and $A, B \in \hat{\mathcal{G}}(n)$. If $\phi(A) = B$ then $\phi(\mathcal{P}_A) = \mathcal{P}_B$.*

Proof. Suppose $\phi(A) = B$. Note that $X \in \mathcal{P}_A$ if and only if there exists some $\delta > 0$ such that $A \pm \epsilon X \in \hat{\mathcal{G}}(n)$. But $A \pm \epsilon X \in \hat{\mathcal{G}}(n)$ if and only if $\phi(A \pm \epsilon X) \in \hat{\mathcal{G}}(n)$. But $\phi(A \pm \epsilon X) = \phi(A) \pm \epsilon\phi(X) = B \pm \epsilon\phi(X)$. Thus $X \in \mathcal{P}_A$ if and only if $\phi(X) \in \mathcal{P}_B$. □

Lemma 2.36 *If $\phi : [\hat{\mathcal{G}}(n)] \to [\hat{\mathcal{G}}(n)]$ is a linear mapping such that $\phi(\hat{\mathcal{G}}(n)) = \hat{\mathcal{G}}(n)$ then $\phi(\mathcal{P}_k) = \mathcal{P}_k$.*

Proof. Using the linearity of ϕ and Lemma 2.35, we see that $\dim \mathcal{P}_A = \dim \phi(\mathcal{P}_A) = \dim \mathcal{P}_{\phi(A)}$. Therefore, is $A \in \mathcal{P}_k$, then $\phi(A) \in \mathcal{P}_k$. Since $\phi(\hat{\mathcal{G}}(n)) = \hat{\mathcal{G}}(n)$ and $\hat{\mathcal{G}}(n) = \bigcup \mathcal{P}_k$, therefore $\phi(\mathcal{P}_k) = \mathcal{P}_k$. □

We use the following lemma in the proof of the main theorem of this section.

Lemma 2.37 *Let $n = 2m$. If $\phi : [\hat{\mathcal{G}}(n)] \to [\hat{\mathcal{G}}(n)]$ is a linear map such that $\phi(\hat{\mathcal{G}}(n)) = \hat{\mathcal{G}}(n)$, then $\phi(\mathcal{C}_k) = \mathcal{C}_k$ for $k = 1, ..., m$. In particular, $\phi(\mathcal{C}_1) = \mathcal{C}_1$.*

Proof. Define

$$r_k = \frac{k(k+1)}{2} + 1 - k = \frac{k(k-1)}{2} + 1.$$

Note that by definition, $\mathcal{C}_k \subseteq \mathcal{P}_{r_k}$, but that $\mathcal{C}_j \bigcap \mathcal{P}_{r_k} = \emptyset$ whenever $j \neq k$. Therefore, by Proposition 2.34,

$$\overline{\mathcal{C}_{k+1}} \bigcap \mathcal{P}_{r_k} = (\mathcal{C}_{k+1} \bigcup \mathcal{C}_k \bigcup \cdots \bigcup \mathcal{C}_1 \bigcup \mathcal{C}_0) \bigcap \mathcal{P}_{r_k} = \mathcal{C}_k.$$

Note that if $\phi(\mathcal{C}_{k+1}) = \mathcal{C}_{k+1}$, then by linearity $\phi(\overline{\mathcal{C}_{k+1}}) = \overline{\mathcal{C}_{k+1}}$. Since $\phi(\mathcal{P}_{r_k}) = \mathcal{P}_{r_k}$ by Lemma 2.36, therefore if $\phi(\mathcal{C}_{k+1}) = \mathcal{C}_{k+1}$, then $\phi(\mathcal{C}_k) = \mathcal{C}_k$. In particular, we will show that $\phi(\mathcal{C}_m) = \mathcal{C}_m$ and therefore $\phi(\mathcal{C}_1) = \mathcal{C}_1$. First, note that $\mathcal{C}_m \subseteq \mathcal{P}_{r_m}$. We now show that $\mathcal{P}_{r_m} \subseteq \mathcal{C}_m$. Since the dimensions of $\mathcal{P}_A$ are the same for elements in these two set, we need only show that if $A \in \mathcal{P}_{r_m}$, then rank $A = m$. Suppose $A \in \mathcal{P}_{r_m}$. If rank $A = k < m$, then the dimension of $\mathcal{P}_A$ is $\frac{k(k+1)}{2} + 1 - k < \frac{m(m+1)}{2} + 1 - m$, so A is not in $\mathcal{P}_{r_m}$. Suppose rank $A = k > m$. Then the smallest possible dimension of $\mathcal{P}_A$ is

$$\frac{k(k+1)}{2}+1-2m \geq \frac{(m+1)(m+2)}{2}+1-2m = \frac{m(m+1)}{2}+2-m > \frac{m(m+1)}{2}+1-m.$$

Therefore, A is not an element of $\mathcal{P}_{r_m}$. And hence, $\mathcal{P}_{r_m} = \mathcal{C}_m$, and so $\phi(\mathcal{C}_m) = \mathcal{C}_m$. Hence $\phi(\mathcal{C}_1) = \mathcal{C}_1$. □

Recall that $\hat{\mathcal{G}}_1(n) = \mathcal{C}_1$. Thus if $\phi(\mathcal{C}_1) = \mathcal{C}_1$, then $\phi(\hat{\mathcal{G}}_1) = \hat{\mathcal{G}}_1$.

Theorem 2.38 *Suppose $n = 2m$. Let $\phi : [\hat{\mathcal{G}}(n)] \to [\hat{\mathcal{G}}(n)]$ be a linear map. Then, for $n > 4$, $\phi(\hat{\mathcal{G}}(n)) = \hat{\mathcal{G}}(n)$ if and only if there exists a permutation matrix P such* *that ϕ has the form*

$$X \mapsto \gamma P X P^t.$$

For $n = 4$, $\phi(\hat{\mathcal{G}}(n)) = \hat{\mathcal{G}}(n)$ if and only if there exists a basis $\{X_1, X_2, X_3\}$ of $[\hat{\mathcal{G}}(4)]$ and scalars $\gamma_1, \gamma_2, \gamma_3 > 0$ and a permutation σ such that ϕ has the form

$$X \mapsto \sum_{i=1}^{3} \alpha_i \gamma_i X_{\sigma(i)}$$

where $X = \sum \alpha_i X_i$.

We will give an outline of the proof. Note that ($\Leftarrow$) is clear. For ($\Rightarrow$), we use the fact that $\phi(\hat{\mathcal{G}}_1) = \hat{\mathcal{G}}_1$ by Lemma 2.37.

First, we define the set $\mathcal{T} = \hat{\mathcal{G}}_1 \bigcap \{A \in \hat{\mathcal{G}}(n) : \operatorname{tr} A = n\}$ and show that it is finite of order $t = \frac{n!}{2(m!)(m!)}$. We label the elements $X_1, \ldots, X_t$ and let $x_1, \ldots, x_t$ be the vectors such that $x_i x_i^t = X_i$ and note that each x_i has m 1s and m -1s. Because ϕ is linear, $\phi(X_i) = \gamma_i X_{\sigma(i)}$ for some permutation σ. Also, $\sum_{i=1}^t X_i = \frac{t}{n-1}(nI_n - J_n)$.

We next show that for $n > 4$, $\gamma_i = \gamma_j$ for all i, j. To do this, we assume γ_k is the largest such scalar and replace ϕ with $\frac{1}{\gamma_k}\phi$. We show that because

$$0 \leq \phi(\sum_{i=1}^{t} X_i - \frac{t}{n-1} X_k) = \sum_{i=1}^{t} \gamma_i X_{\sigma(i)} - \frac{t}{n-1} X_{\sigma(k)},$$

therefore

$$0 \leq x_{\sigma(k)}^t (\sum_{i=1}^{t} \gamma_i X_{\sigma(i)} - \frac{t}{n-1} X_{\sigma(k)}) x_{\sigma(k)} = 0$$

. This implies that $\gamma_i = 1$ whenever $(x_{\sigma(k)}^t x_{\sigma(i)}) \neq 0$. Repeating this argument shows $\gamma_i = 1$ for all i. This gives us that $\phi(\mathcal{T}) = \mathcal{T}$ and $\phi(nI - J) = nI - J$.

Next, we show that ϕ preserves inner product on $\mathcal{T}$ by grouping together those X_i and X_j such that, for different values of α and β, $\beta(nI - J) - X_i - \alpha X_j$ and therefore $\beta(nI - J) - X_{\sigma(i)} - \alpha X_{\sigma(j)}$ is positive semidefinite.

We now begin the process of replacing ϕ with the mapping $X \mapsto P\phi(X)P^t$ in a sucessive manner, each time adding at least one element of $X \in \mathcal{T}$ such that $\phi(X) = X$. We first choose the element $X_1 \in \mathcal{T}$ and let P_1 be such that $X_1 = P_1 X_{\sigma(1)} P_1^t$. Replace ϕ with $X \mapsto P_1\phi(X)P_1^t$. Because ϕ preserves inner product, we can find subsets of $\mathcal{T}$ that are mapped to themselves, defined by their inner product with X_1. By a judicious choose of X_2 (relabelling as necessary), we can find a permutation matrix P_2 such that $P_2 X_1 P_2^t = X_1$ and $X_2 = P_2 X_{\sigma(2)} P_2^t$. Replace ϕ with $X \mapsto P_2\phi(X)P_2^t$. Repeat this process with an appropriate X_3 andP_3 to get $\phi(X_i) = X_i$ for $i = 1, 2, 3$. This is sufficient to show that $\phi(X) = X$ for all $X \in \mathcal{T}$. Because ϕ is linear, this implies $\phi(X) = X$ for all $X \in \hat{\mathcal{G}}_1$. Because $\hat{\mathcal{G}}_1$ spans $[\hat{\mathcal{G}}(n)]$, ϕ is the identity map. This implies that the original ϕ will be of the desired form for $n > 4$.

For $n = 4$, note that $\mathcal{T} = \{X_1, X_2, X_3\}$ is a linearly independent set. This problem is similar to one in which you map the positive octant of a 3–dimensional Euclidean space back to itself. Each of the axes are mapped to another axis with a scaling factor. In other words, there is a permutation σ of $(1, 2, 3)$ associated with ϕ such that $\phi(X_i) = \gamma_i X_{\sigma(i)}$. Recalling that ϕ is linear, we see that ϕ will have the desire form.

As we have only shown the form of preservers of $\hat{\mathcal{G}}(n)$ for when n is even, we can only find the form of linear mappings $\psi : [\hat{\mathcal{D}}(n)] \to [\hat{\mathcal{D}}(n)]$ such that $\psi(\hat{\mathcal{D}}(n)) = \hat{\mathcal{D}}(n)$.

Theorem 2.39 *Suppose $n = 2m$. Let $\psi : [\hat{\mathcal{D}}(n)] \to [\hat{\mathcal{D}}(n)]$ be a linear map. Then $\psi(\hat{\mathcal{D}}(n)) = \hat{\mathcal{D}}(n)$ if and only if there exists a permutation matrix P such that ψ has the form*

$$X \mapsto \gamma P X P^t$$

for $n > 4$ and

$$X \mapsto D P X P^t D^t$$

for $n = 4$, where D is a diagonal scaling.

Proof. Note that $\psi(\hat{\mathcal{D}}(n)) = \hat{\mathcal{D}}(n)$ if and only if $\psi \circ \kappa(\hat{\mathcal{G}}(n)) = \kappa(\hat{\mathcal{G}}(n))$ if and only if $\tau \circ \psi \circ \kappa(\hat{\mathcal{G}}(n)) = \hat{\mathcal{G}}(n)$. From Theorem 2.38, if $n > 4$, then $\psi(\hat{\mathcal{D}}(n)) = \hat{\mathcal{D}}(n)$ if and only if there exists a permutation matrix P and $\gamma > 0$ such that

$$\tau \circ \psi \circ \kappa(X) = \gamma P X P^t.$$

Applying κ to both sides of the above equation, and choosing $Y \in \hat{\mathcal{D}}(n)$ such that $\kappa(X) = Y$, we obtain

$$\begin{aligned}
\psi(Y) &= \psi \circ \kappa(X) = \kappa(\gamma P X P^t) = \kappa(\gamma P \tau(Y) P^t) \\
&= -\frac{1}{2}\kappa\left(\gamma P \left(I - \frac{1}{n}J\right) Y \left(I - \frac{1}{n}J\right) P^t\right) \\
&= -\frac{1}{2}\kappa\left(\gamma \left(I - \frac{1}{n}J\right) P Y P^t \left(I - \frac{1}{n}J\right)\right) = \kappa \circ \tau(\gamma P Y P^t) = \gamma P Y P^t
\end{aligned}$$

because $PYP^t \in \hat{\mathcal{D}}(n)$ if and only if $\hat{\mathcal{D}}(n)$. If $n = 4$, then $\psi(\hat{\mathcal{D}}(n)) = \hat{\mathcal{D}}(n)$ if and only if there exists the basis $\{X_1, X_2, X_3\}$, scalars $\gamma_1, \gamma_2, \gamma_3 > 0$ and permutation σ

such that

$$\tau \circ \psi \circ \kappa(X) = \sum_{i=1}^{3} \alpha_i \gamma_i X_{\sigma(i)}$$

where $X = \sum \alpha_i X_i$. As before, applying κ to both sides and letting $Y_i = \kappa(X_i)$ and $Y = \kappa(X)$, we obtain

$$\begin{aligned} \psi(Y) &= \psi \circ \kappa(X) = \kappa(\sum_{i=1}^{3} \alpha_i \gamma_i X_{\sigma(i)}) \\ &= \kappa(\sum_{i=1}^{3} \alpha_i \gamma_i \tau(Y_{\sigma(i)})) \\ &= \kappa(\tau(\sum_{i=1}^{3} \alpha_i \gamma_i Y_{\sigma(i)})) = \sum_{i=1}^{3} \alpha_i \gamma_i Y_{\sigma(i)} \end{aligned}$$

because τ is linear and $\sum \alpha_i \gamma_i Y_{\sigma(i)} \in \hat{\mathcal{D}}(4)$. □

The proof of Theorem 2.38 (for $n > 4$) relied on the fact that we could find a set $\mathcal{T}$ that was finite, spanned $[\hat{\mathcal{G}}(n)]$ and had the property that it could be shown that $\phi(\mathcal{T}) = \gamma \mathcal{T}$. We then showed that $\phi(X) = \gamma P X P^t$ for all $X \in \mathcal{T}$. This was sufficient to show that ϕ had the desired form. In the odd case, we would like to find such a $\mathcal{T}$. For n odd, we tried numerous approaches similar to the even case, but each time, were unable to find a useful finite subset. It is our belief that a new approach will be necessary to solve this problem for n odd.

Chapter 3

Ray-Nonsingular Matrices

3.1 Introduction

A complex matrix is a *ray-pattern matrix* if all of its nonzero entries have modulus 1. A ray-pattern matrix is *full* if each of its entries is nonzero. An $n \times n$ complex matrix A is *ray-nonsingular* if $A \circ X$ is nonsingular for all entry-wise positive matrices X. Ray-nonsingular matrices with real entries are known as *sign-nonsingular* matrices; see [39] and its references. In [39], the authors posed the following question:

For which n does there exist a full $n \times n$ ray-nonsingular matrix?

It is not hard to construct examples of full $n \times n$ ray-nonsingular matrices for $n \leq 4$; see [30, 39]. In [30], the authors showed that there are no full $n \times n$ ray-nonsingular matrices for $n \geq 6$. The question of whether there are full 5×5 ray-nonsingular matrices remained open. In this section, we show that no full 5×5 ray-pattern matrix is ray-nonsingular. As a result, we have the following complete answer for the question raised in [39]:

Main Theorem *There is a full $n \times n$ ray-nonsingular matrix if and only if $n \leq 4$.*

The proof of the main theorem is quite detailed. In section 2, we recall some known results and outline our strategy for the proof. The key to the proof is an understanding of 3 by 3 ray-patterns that are not ray-nonsingular. These are studied in section 3. The proof of the main theorem is given in section 4.

3.2 Preliminary Results and Strategies of Proof

We first recall some terminology from [30]. A nonzero, diagonal ray-pattern matrix is a called a *complex signing.* A complex signing is *strict* if all diagonal entries are nonzero. A $(1,-1)$-*signing* is a diagonal matrix with diagonal entries in $\{1,-1\}$. A vector v is *balanced* if zero is in the relative interior of the convex hull of $\{v_i : 1 \leq i \leq n\}$. Furthermore, it is *strongly balanced* if its entries take on at least three distinct values. A ray-pattern vector v is *generic* if for all $i < j$, $v_i \neq \pm v_j$.

Consider the relation on the set of ray-patterns defined by $A \sim B$ if and only if there exist matrices P and Q, each a product of permutation matrices and complex signings, such that $B = P\hat{A}Q$ where $\hat{A} = A$, A^t or $\overline{A}$. Clearly, $\sim$ is an equivalence relation, and we have the following observation.

Lemma 3.1 *Suppose A and B are full ray-pattern matrices with $A \sim B$. Then A is ray-nonsingular if and only if B is ray-nonsingular.*

We say that the matrix A is *strongly balanceable* if $A \sim B$ for some B each of whose columns is strongly balanced. The following three lemmas from [30] will be useful in establishing the nonexistence of a 5×5 full ray-nonsingular matrix.

Lemma 3.2 [30, Lemma 3.7] *Let $A = (a_{ij}) \in M_n$ be a ray-pattern matrix. If A has an $m \times m$ strongly balanceable submatrix with $m \geq 3$, then A is not ray-nonsingular.*

In section 3, we establish sufficient conditions for a 3 by 3 full ray-pattern to be strongly balanceable.

Lemma 3.3 [30, Theorem 4.3] *Let $A = (a_{ij}) \in M_5$ be a full ray-pattern. If $a_{ij} \in \{1, -1, i, -i\}$, then A is not ray-nonsingular.*

Lemma 3.4 [30, Proposition 4.4] *Let A be a full 5×5 ray-pattern matrix with first column consisting of all 1's and each remaining column generic. Then A is not ray-nonsingular.*

Note that Lemma 3.4 implies that if A is a full 5×5 ray-nonsingular matrix, then each row and column of A intersects a 2×2 submatrix of the form

$$\begin{bmatrix} x & y \\ z & \pm yz/x \end{bmatrix}.$$

Otherwise we can find some $B \sim A$ with the first column all 1's and the last four columns generic.

General strategy of proof. We now give a basic outline of our strategy for proving the main theorem. The proof will be by contradiction. Thus, we will assume to the contrary that there is a full 5 by 5 ray-nonsingular matrix $A = (a_{ij})$. We then use the results of section 3 (that give sufficient conditions for a full 3 by 3 ray-pattern to be strongly balanceable) and Lemmas 3.1–3.4 to show that, up to $\sim$ equivalence, the leading 3×3 submatrix of A has one of the following forms:

$$\text{(a)} \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & e^{i\alpha} & e^{i\beta} \end{bmatrix}, \quad \text{(b)} \begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & e^{i\alpha} & e^{i\beta} \end{bmatrix}, \quad \text{(c)} \begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & e^{i\beta} \\ 1 & e^{i\alpha} & -1 \end{bmatrix},$$

$$\text{(d)} \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & e^{i\beta} \\ 1 & e^{i\alpha} & -1 \end{bmatrix}, \quad \text{or} \quad \text{(e)} \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & e^{i\beta} \\ 1 & e^{i\alpha} & 1 \end{bmatrix}.$$

Next, for each of these cases, we use Lemma 3.3 and the results of section 3 to conclude that either

(i) all entries of A belong to $\{1, -1, i, -i\}$, or

(ii) all entries of A belong to $\{1, e^{2\pi i/3}, e^{4\pi i/3}\}$ arranged in certain patterns.

Finally, we obtain a contradiction by showing that if A satisfies (i) or (ii), then A is not ray-nonsingular.

3.3 Sufficient Conditions for 3×3 Patterns to be Strongly Balanceable

One of the keys to our proof of the main theorem is Lemma 3.2 which asserts that no 3×3 submatrix of a 5×5 ray-nonsingular matrix is strongly balanceable. In this section, we give sufficient conditions for a full 3×3 ray pattern to be strongly balanceable.

By Lemma 3.1, we may restrict our attention to ray-patterns B of the form

$$B = \begin{bmatrix} 1 & 1 & 1 \\ 1 & e^{i\alpha_2} & e^{i\beta_2} \\ 1 & e^{i\alpha_3} & e^{i\beta_3} \end{bmatrix}. \tag{3.3.1}$$

As the function e^{ix}, x real, is 2π-periodic, we may assume that each of α_2, α_3, β_2 and β_3 lies in the interval $(-\pi, \pi]$. For convenience we partition $(-\pi, \pi]$ by the following sets:

$$\mathcal{P} = (0, \pi), \quad \mathcal{N} = (-\pi, 0), \quad \{0\}, \quad \{\pi\},$$

We first determine the strict signings S for which the vector $(1, 1, 1)S$ is strongly balanced. Note that for each $\theta \in (-\pi, \pi]$, the vector $(1, 1, 1)S$ is strongly balanced if and only if the vector $(1, 1, 1)(e^{i\theta}S)$ is strongly balanced. Hence, it suffices to determine the S whose leading diagonal entry is 1.

Lemma 3.5 *Let $S = diag(1, e^{ix}, e^{iy})$ be a strict signing with $x, y \in (-\pi, \pi]$. Then $(1, 1, 1)S$ is strongly balanced if and only if $x \in \mathcal{P}$ and $-\pi < y \leq x - \pi$, or $x \in \mathcal{N}$ and $\pi + x < y < \pi$.*

Proof. Note that $(1,1,1)S$ is strongly balanced if and only if no two of 1, e^{ix} and e^{iy} are equal or opposite, and the convex hull, H, of $\{1, e^{ix}, e^{iy}\}$ contains the origin. Thus, $(1,1,1)S$ is not strongly balanced if $x = 0$, $x = \pi$, $y = 0$, $y = \pi$ or $x = \pm y$. If $x \in \mathcal{P}$, then it is easy to verify that H contains the origin if and only if $-\pi < y \leq x - \pi$. If $x \in \mathcal{N}$, then it is easy to verify that H contains the origin if and only if $\pi + x < y < \pi$. The lemma now follows. ■

The shaded regions without their boundaries given in Figure 3.1, represent the region of the Cartesian plane determined by the inequalities in Lemma 3.5.

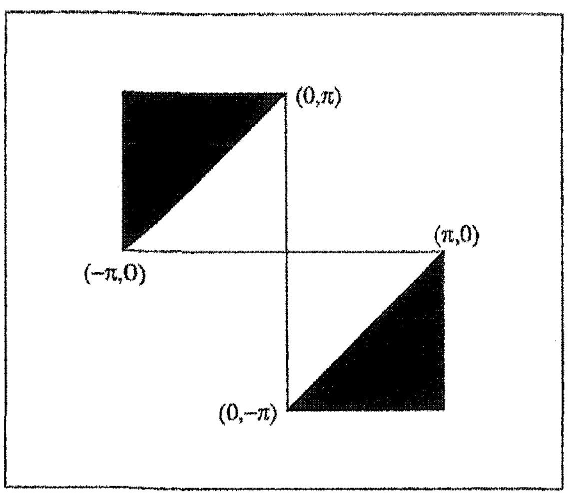


Figure 3.1: Graphical representation of solution set balancing $[1,1,1]$

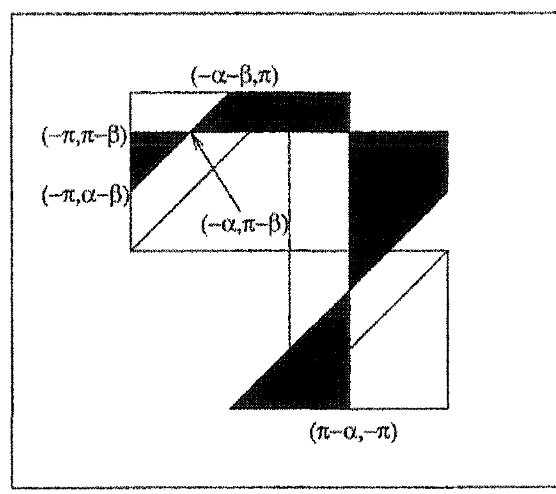


Figure 3.2: Graphical representation of shifted solution set balancing $[1, e^{i\alpha}, e^{i\beta}]$ with $0 < \beta < \alpha < \pi$

Next, let's investigate a general vector $z = (1, e^{i\alpha}, e^{i\beta})$, and let $R(\alpha, \beta)$ be the region of the Cartesian plane consisting of the points (x, y) such that $z\text{diag}(1, e^{ix}, e^{iy})$ is strongly balanced and $x, y \in (-\pi, \pi]$. Thus $R(0,0)$ is the region described in

Lemma 1, and illustrated in Figure 3.1. Let $D = \text{diag}(1, e^{i\alpha}, e^{i\beta})$. Note that S is a strict signing such that zS is strongly balanced if and only if DS is a strict signing such that $(1,1,1)DS$ is strictly balanced. It follows that $R(\alpha,\beta)$ can be obtained from $R(0,0)$ by identifying opposite edges of the square $[-\pi,\pi]\times[-\pi,\pi]$ to form a torus, and then translating the shaded region in Figure 3.1 by $(-\alpha,-\beta)$.

For example, $R(\alpha,\beta)$ is presented as the shaded region in Figure 3.2 where $\alpha,\beta \in (0,\pi)$ and $\alpha > \beta$.

Note that $R(0,0)\cap R(\alpha,\beta)$ represents the points (x,y) in the plane such that both rows of

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & e^{i\alpha} & e^{i\beta} \end{bmatrix} \text{diag}(1, e^{ix}, e^{iy})$$

are strongly balanced.

It is tedious, but straightforward, to determine the regions $R(0,0)\cap R(\alpha,\beta)$. We do this as follows. First partition the vectors of the form $z = \begin{bmatrix} 1 & e^{i\alpha} & e^{i\beta} \end{bmatrix}$ according to the locations and relationships between α and β as given by the 24 classes described in Table 3.1 below. The sets $R(0,0)\cap R(\alpha,\beta)$ for each of these 24 cases are the shaded regions without the boundaries illustrated in Section 5.

We finally turn our attention to studying the strong balanceability of the matrix B in (3.3.1). Note that B is strongly balanceable if and only if $R(0,0)\cap R(\alpha_2,\beta_2)\cap R(\alpha_3,\beta_3)\neq\emptyset$, or equivalently if and only if $(R(0,0)\cap R(\alpha_2,\beta_2))\cap(R(0,0)\cap R(\alpha_3,b_3))\neq\emptyset$. If the second (or third) row has form (C9) in Table 3.1, i.e. is $[1,1,1]$, then trivially, this intersection corresponds to the solution set of the first and third

Table 3.1: Classes of vectors of the form $[1\, e^{i\alpha}\, e^{i\beta}]$.

Class	α in	β in	Conditions
1	$(0,\pi)$	$(0,\pi)$	$\alpha > \beta$
2	$(0,\pi)$	$(0,\pi)$	$\alpha < \beta$
3	$(-\pi,0)$	$(-\pi,0)$	$\alpha > \beta$
4	$(-\pi,0)$	$(-\pi,0)$	$\alpha < \beta$
5	$(0,\pi)$	$(-\pi,0)$	$\alpha - \beta < \pi$
6	$(0,\pi)$	$(-\pi,0)$	$\alpha - \beta > \pi$
7	$(-\pi,0)$	$(0,\pi)$	$\beta - \alpha < \pi$
8	$(-\pi,0)$	$(0,\pi)$	$\beta - \alpha > \pi$
9	$(0,\pi)$	$(0,\pi)$	$\alpha = \beta$
10	$(-\pi,0)$	$(-\pi,0)$	$\alpha = \beta$
11	$(0,\pi)$	$(-\pi,0)$	$\alpha - \beta = \pi$
12	$(-\pi,0)$	$(0,\pi)$	$\beta - \alpha = \pi$

Class	α in	β in
C1	$(0,\pi)$	$\{0\}$
C2	$(-\pi,0)$	$\{0\}$
C3	$(0,\pi)$	$\{\pi\}$
C4	$(-\pi,0)$	$\{\pi\}$
C5	$\{0\}$	$(0,\pi)$
C6	$\{0\}$	$(-\pi,0)$
C7	$\{\pi\}$	$(0,\pi)$
C8	$\{\pi\}$	$(-\pi,0)$
C9	$\{0\}$	$\{0\}$
C10	$\{0\}$	$\{\pi\}$
C11	$\{\pi\}$	$\{0\}$
C12	$\{\pi\}$	$\{\pi\}$

(or second) row. Also, if the second (or third) row has form (C10)-(C12), then the solution set is empty (see Figure 3.24) and so the intersection is trivially empty. Thus, we need only consider those cases when the second and third rows are of one of the first 20 types listed on Table 3.1. That is, we need to study the intersection of $(R(0,0) \cap R(\alpha_2, \beta_2))$ and $(R(0,0) \cap R(\alpha_3, b_3))$ for pairs of the first 20 classes listed in Table 3.1.

The results of this straight-forward but tedious study are summarized in Table 3.2 found at the end of Section 3.5. The rows and columns of Table 3.2 are indexed by the 20 classes other than (C9)-(C12). An entry of '1' indicates that the pair of specified regions always has nonempty intersection, an entry '$\emptyset$' indicates that the pair of specified regions always has an empty intersection, and an entry 'c' indicates that the intersection is empty or nonempty depending on the values of $\alpha_2, \alpha_3, \beta_2, \beta_3$.

Table 3.3 will list the conditions on the values of $\alpha_2, \alpha_3, \beta_2, \beta_3$ for an empty intersection corresponding to some of the 'c's in Table 3.2.

The following example illustrates how we obtain the conditions in Table 3.3.

Example 3.6 Consider the matrix B in (3.3.1). Let u_1, u_2, u_3 be the rows of B. Suppose that u_2 has form (C5) and u_3 has form (C1). Since we are interested in the conditions on β_2 and α_3 such that the matrix is not strongly balanced, we examine when the solution sets described geometrically above do not intersect. In the upper left quadrant, we see that the upper bound for (C5) is $\pi - \beta_1$ while the lower bound for (C1) is α_2, thus $\pi - \beta_1 \leq \alpha_2$. When we examine the lower right quadrant, we get the same inequality.

Next, we illustrate how to use Tables 3.2 and 3.3 to examine specific matrices. This will allow the reader to get a feel for how these arguments work while also providing information needed latter.

Example 3.7 Suppose u_1, u_2, u_3 are rows of B with

$$u_1 = [\ 1 \quad 1 \quad 1\ ], \quad u_2 = [\ 1 \quad 1 \quad e^{i\beta_1}\ ], \quad u_3 = [\ 1 \quad -1 \quad e^{i\beta_2}\ ],$$

with $\{e^{i\beta_1}, e^{i\beta_2}\} \cap \{\pm 1\} = \emptyset$, so that B cannot be strongly balanced. If we assume that $\beta_1 \in \mathcal{P}$, then u_2 has form (C5) and u_3 has form (C7) or (C8). By Table 3.3, if u_3 has form (C7) then $\beta_2 \leq \beta_1$, if u_3 has form (C8), then $\beta_2 + \pi \leq \beta_1$. If we are interested in the vector $v = [\ 1 \quad e^{i\beta_1} \quad e^{i\beta_2}\ ]$, then v has one of the following forms: (1), (6), (9) or (11). Similarly. if $\beta_2 \in \mathcal{N}$, then v has one of the following forms: (4), (8), (10), or (12).

Using a similar analysis, we have the following.

Example 3.8 Suppose u_1, u_2, u_3 are rows of B with

$$u_1 = \begin{bmatrix} 1 & 1 & 1 \end{bmatrix}, \quad u_2 = \begin{bmatrix} 1 & -1 & e^{i\beta_1} \end{bmatrix}, \quad u_3 = \begin{bmatrix} 1 & 1 & e^{i\beta_2} \end{bmatrix},$$

with $\{e^{i\beta_1}, e^{i\beta_2}\} \cap \{\pm 1\} = \emptyset$, so that B cannot be strongly balanced. Then $[1\ e^{i\beta_1}\ e^{i\beta_2}]$ has one of the following forms: (2), (3), (6) or (8)–(12).

3.4 Proof of Main Theorem

Assume A is a 5×5 full ray-nonsingular matrix. We first show that up to the equivalence relation defined before Lemma 3.1, we may assume that the leading 3×3 principle submatrix has one of the following forms.

$$\text{(a)} \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & e^{i\alpha} & e^{i\beta} \end{bmatrix}, \quad \text{(b)} \begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & e^{i\alpha} & e^{i\beta} \end{bmatrix}, \quad \text{(c)} \begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & e^{i\beta} \\ 1 & e^{i\alpha} & -1 \end{bmatrix},$$

$$\text{(d)} \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & e^{i\beta} \\ 1 & e^{i\alpha} & -1 \end{bmatrix}, \quad \text{or} \quad \text{(e)} \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & e^{i\beta} \\ 1 & e^{i\alpha} & 1 \end{bmatrix}.$$

Recall that if $A = (a_{jk})$ is a 5×5 full ray-nonsingular matrix, then each row and column intersects a 2×2 submatrix of the form

$$\begin{bmatrix} x & y \\ z & \pm\frac{yz}{x} \end{bmatrix}.$$

By Lemma 3.1, we may assume that the 2×2 submatrix intersecting the first row lies on the first and second row and column. Likewise, we assume that $a_{jk} = 1$ whenever $j = 1$ or $k = 1$. Then $a_{22} = \pm 1$. Let $a_{jk} = e^{ix_{jk}}$ and $u_j = [1, e^{ix_{j2}}, e^{ix_{j3}}]$ for $j = 1, 2, 3, 4, 5$.

First, suppose $e^{ix_{23}} = \pm 1$ or $e^{ix_{j2}} = \pm 1$ for some $j = 3, 4$ or 5. Then A has a 3×3 submatrix equivalent to a matrix of form (a) or (b). By Lemma 3.1, we can replace A with the equivalent matrix with leading 3×3 principle submatrix of form (a) or (b).

Now suppose, for some $j = 3, 4$ or 5, that $e^{ix_{j3}} = \pm 1$. Then A has a 3×3 submatrix equivalent to a matrix of form (c), (d) or (e). By Lemma 3.1, we can replace A with the equivalent matrix with leading 3×3 principle submatrix of form (c), (d) or (e).

Suppose, for some $j = 3, 4$ or 5, that $e^{ix_{j2}} = \pm e^{ix_{j3}}$. Then

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & \pm 1 & e^{ix_{23}} \\ 1 & e^{ix_{j2}} & \pm e^{ix_{j2}} \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 \\ \pm 1 & 1 & \pm e^{ix_{23}} \\ e^{-ix_{j2}} & 1 & \pm 1 \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 \\ 1 & \pm 1 & \pm e^{ix_{23}} \\ 1 & e^{-ix_{j2}} & \pm 1 \end{bmatrix}.$$

In other words, A has a 3×3 submatrix equivalent to a matrix of form (c), (d) or (e). By Lemma 3.1, we can replace A with the equivalent matrix with leading 3×3 principle submatrix of form (c), (d) or (e).

Now suppose that neither of the two cases above hold. We will then show, using Table 3.2 and the fact that A cannot have a 3×3 strongly balanced submatrix, that no such matrix is possible. Note that by our assumption, u_3, u_4 and u_5 do not have forms (C1) – (C12) nor (9) – (12). Also, u_2 can only have form (C5) – (C8). In fact, since $A \sim \overline{A}$, we may assume that $x_{23} \in \mathcal{P}$, and therefore u_2 has either form (C5) or (C7). Suppose u_2 has form (C5). Because the matrix with rows u_1, u_2 and u_j is not strongly balanced, by Table 3.2, u_j for $j = 3, 4, 5$ can only have form

(1), (4), (6) or (8).

Note that if two vectors, say u_j and u_k, have the same form, then the matrix with rows u_1, u_j and u_k will be strongly balanced by Table 3.2. Now suppose one of the row vectors, say u_3, has form (1). Then u_4 and u_5 both have form (6), else the matrix with rows u_1, u_3 and u_k is strongly balanced, with $k = 4, 5$. But then the matrix with rows u_1, u_4 and u_5 is strongly balanced. So u_3 cannot have form (1). Suppose u_3 has form (4). Then u_4 and u_5 both have form (8), else the matrix with rows u_1, u_3 and u_k is strongly balanced, with $k = 4, 5$. But then the matrix with rows u_1, u_4 and u_5 is strongly balanced. So u_3 cannot have form (4). Thus we have three vectors and only two possible forms, so two vectors have the same form and we have a strongly balanced 3×3 submatrix. Thus, u_2 cannot have form (C5). Now, suppose u_2 has form (C7). Because the matrix with rows u_1, u_2 and u_j is not strongly balanced, by Table 3.2, u_j for $j = 3, 4, 5$ can only have form

(2), (5) or (6).

As no form can be repeated, we can assume that u_3 has form (2), u_4 has form (5) and u_5 has form (6). But then the matrix with rows u_1, u_3 and u_5 is strongly balanced by Table 3.2. Therefore, u_2 cannot have form (C7) and we have a contradiction.

3.4.1 Case 1

First we assume that the leading 3×3 principal submatrix of A has form (a). Suppose u_1, u_2, u_3, u_4, u_5 are the five rows of $[a_{ij}]_{1 \le i \le 5, 1 \le j \le 3}$. Then $u_1 = u_2 = [\ 1 \quad 1 \quad 1\ ]$. Let

$$u_3 = [\ 1 \quad e^{i\alpha_3} \quad e^{i\beta_3}\ ], \quad u_4 = [\ 1 \quad e^{i\alpha_4} \quad e^{i\beta_4}\ ], \quad u_5 = [\ 1 \quad e^{i\alpha_5} \quad e^{i\beta_5}\ ].$$

Note that for $i = 3, 4, 5$, u_i cannot be of the form (1)–(12) or (C1)–(C8); otherwise the matrix with rows u_1, u_2, u_i can be strongly balanced by Table 3.2. So u_i has form (C10), (C11) or (C12). If $u_3 = u_4 = u_5$, then the matrix with rows u_3, u_4, u_5 can be strongly balanced. Suppose u_3, u_4, u_5 are not all equal. Then up to the equivalence relation $\sim$ described after Lemma 3.1, we may assume that A is equal to one of the following two matrices.

$$B_1 = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & a_{24} & a_{25} \\ 1 & 1 & -1 & a_{34} & a_{35} \\ 1 & 1 & -1 & a_{44} & a_{45} \\ 1 & -1 & 1 & a_{54} & a_{55} \end{bmatrix}, \qquad B_2 = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & a_{24} & a_{25} \\ 1 & 1 & -1 & a_{34} & a_{35} \\ 1 & -1 & -1 & a_{44} & a_{45} \\ 1 & -1 & 1 & a_{54} & a_{55} \end{bmatrix}$$

In both cases, A has the 3×3 submatrices

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & a_{2j} \\ 1 & 1 & a_{3j} \end{bmatrix} \text{ and } \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & a_{2j} \\ 1 & 1 & a_{5j} \end{bmatrix}$$

for $j = 4,5$. So $a_{ij} = \pm 1$ for $i = 2,3,5$ and $j = 4,5$. If $A = B_1$, then A has the 3×3 submatrices

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & a_{2j} \\ 1 & 1 & a_{4j} \end{bmatrix},$$

and so $a_{4j} = \pm 1$ for $j = 4,5$. If $A = B_2$, then A has the 3×3 submatrices

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & a_{2j} \\ -1 & -1 & a_{4j} \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & a_{2j} \\ 1 & 1 & -a_{4j} \end{bmatrix}.$$

Thus, $a_{4j} = \pm 1$ for $j = 4,5$. And therefore, $a_{ij} = \pm 1$ for all i, j, and by Lemma 3.3 (a), A is not ray-nonsingular.

3.4.2 Case 2

Assume that the leading 3×3 principal submatrix of A has form (b). We will show that A has entries $a_{ij} \in \{\pm 1, \pm i\}$, which contradicts Lemma 3.3 (a).

Suppose $u_1, \ldots, u_5$ are the five rows of $[a_{ij}]_{1 \le i \le 5, 1 \le j \le 3}$. Then $u_1 = [1\ 1\ 1]$ and $u_2 = [1\ -1\ 1]$, i.e. they have forms (C9) and (C11) respectively. Let

$$u_3 = [\ 1 \quad e^{ix_3} \quad e^{iy_3}\ ], \quad u_4 = [\ 1 \quad e^{ix_4} \quad e^{iy_4}\ ], \quad u_5 = [\ 1 \quad e^{ix_5} \quad e^{iy_5}\ ].$$

Since for each $j \in \{3,4,5\}$ the matrix with rows u_1, u_2, u_j cannot be strongly balanced, using A^t and Example 3.8 we see that u_j has one of the following forms:

(2), (3), (6), (8) – (12), (C3) – (C8), (C10) or (C11).

Note that if $e^{iy_j} = 1$ for any $j = 3,4,5$, then A is equivalent to a matrix with a submatrix of form (a), and we are back to Case 1. Similarly, if $e^{iy_j} = -1$ for all $j = 3,4,5$, then A is equivalent to a matrix with a 3×3 submatrix of form (a) and we are back to case 1. So there exists a $j \in \{3,4,5\}$ such that $e^{iy_j} \neq \pm 1$. We may assume $y_3 \in \mathcal{P}$ since $A \sim \overline{A}$. By this assumption, we see that u_3 will be of the following forms:

$$(2), (8), (9), (12), (C5) \text{ or } (C7).$$

Next, let $v_1, \ldots, v_5$ be the rows of the matrix obtained from $[a_{ij}]_{1 \le i \le 5, 1 \le j \le 3}$ by multiplying -1 to its second column. Then

$$v_1 = [1\ -1\ 1],\ v_2 = [1\ 1\ 1],\ v_3 = [1\ -e^{ix_3}\ e^{iy_3}],\ v_4 = [1\ -e^{ix_4}\ e^{iy_4}],\ v_5 = [1\ -e^{ix_5}\ e^{iy_5}].$$

Note that u_3 has form (2), (9), (C5) if and only if v_3 has form (8), (12), (C7), respectively. Thus, we may assume that u_3 has form

$$(2), (9) \text{ or } (C5)$$

otherwise, multiply the second column of A by -1, and interchange the first two rows of the resulting matrix. Now, we consider several subcases.

A. Assume either u_4 or u_5 has form (C10) or (C12). In particular, we may assume that u_5 has form (C10) or (C12); otherwise we permute the fourth and fifth row of A.

A.i. Suppose $u_5 = [1, 1, -1]$ has form (C10). Recall that u_3 has form (2), (9) or (C5) while u_4 has one of the forms: (2), (3), (6), (8), (9)–(12), (C3)–(C8), (C10) or (C12).

Suppose u_3 has form (C5). But then

$$\begin{bmatrix} u_1 \\ u_5 \\ u_3 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 1 & 1 & e^{iy_3} \end{bmatrix}$$

is equivalent to a matrix of the form in Case 1.

Next, consider the matrix

$$\begin{bmatrix} u_1 \\ u_5 \\ u_j \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 1 & e^{ix_j} & e^{iy_j} \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & e^{ix_j} \\ 1 & -1 & e^{iy_j} \end{bmatrix}$$

for $j = 3, 4$. Since this submatrix is not strongly balanced, by Example 3.7, u_3 cannot have form (2). Hence it has form (9). Furthermore, u_4 cannot have form (2) or (3). Also, if u_4 has form (9) or (C10) or if $e^{ix_4} = 1$, then there is a submatrix of the form in Case 1.

Note that

$$\begin{bmatrix} u_2 \\ u_5 \\ u_4 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 \\ -1 & 1 & e^{ix_4} \\ 1 & -1 & e^{iy_4} \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & -e^{ix_4} \\ 1 & -1 & e^{iy_4} \end{bmatrix}.$$

From Table 3.2, we see that if the above matrix is not strongly balanced and $e^{ix_j}, e^{iy_j} \neq \pm 1$, then the sign of the imaginary parts of $-e^{ix_j}$ and e^{iy_j} do not agree. In other words, $x_j \in \mathcal{P}$ implies $y_j \in \mathcal{P}$ and $x_j \in \mathcal{N}$ implies $y_j \in \mathcal{N}$. So u_4 can only have form (10), (C3), (C4), (C7), (C8) or (C12).

If u_4 has form (10), then the matrix formed by rows u_1, u_3, u_4 is equivalent to

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & e^{ix_3} & e^{ix_3} \\ 1 & e^{ix_4} & e^{ix_4} \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 \\ e^{-ix_3} & 1 & 1 \\ e^{-ix_4} & 1 & 1 \end{bmatrix},$$

and again we are back to Case 1. If u_4 has form (C3), then note that v_3 has form (11) and v_4 has form (C4) and so the matrix with rows v_2, v_3, v_4 is strongly balanced. The vector u_4 cannot have forms (C4) or form (C8) else the matrix with rows u_1, u_3, u_4 is strongly balanced. Likewise, u_4 cannot have form (C7); otherwise, for some $x_3, y_4 \in \mathcal{P}$, the matrix with rows u_5, u_3, u_4 can be strongly balanced because it is equivalent to

$$\begin{bmatrix} 1 & 1 & -1 \\ 1 & e^{ix_3} & e^{ix_3} \\ 1 & -1 & e^{iy_4} \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 \\ 1 & e^{ix_3} & -e^{ix_3} \\ 1 & -1 & -e^{iy_4} \end{bmatrix}$$

which has rows of form (11) and (C8). If u_4 has form (C12), the matrix with rows u_1, u_3, u_4 is equivalent to

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & e^{ix_3} & e^{ix_3} \\ 1 & -1 & -1 \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 \\ e^{-ix_3} & 1 & 1 \\ -1 & 1 & 1 \end{bmatrix}$$

and we are back to Case 1.

A.ii. Suppose $u_5 = [1, -1, -1]$ has form (C12). Recall that u_3 has form (2), (9) or (C5) while u_4 has one of the following forms: (2), (3), (6), (8), (9)–(12), (C3)–(C8), (C10) or (C12). Suppose u_3 has form (2) or (9). But then

$$\begin{bmatrix} u_1 \\ u_3 \\ u_5 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & e^{ix_3} & e^{iy_3} \\ 1 & -1 & -1 \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 \\ 1 & e^{ix_3} & -1 \\ 1 & e^{iy_3} & -1 \end{bmatrix}$$

can be strongly balanced because the last two rows both have form (C3).

Suppose u_3 has form (C5). Note that if u_4 has form (C10) then we are back to Case A.i. and if it has form (C12) then we have a 3×3 submatrix of form (a) and we are back to Case 1. By Table 3.2, u_4 can only have one of the following forms: (6), (8), (10), (12), (C3), (C6), (C7) or (C8).

Suppose u_4 has either form (6) or (8). Then the matrix

$$\begin{bmatrix} u_5 \\ u_2 \\ u_4 \end{bmatrix} = \begin{bmatrix} 1 & -1 & -1 \\ 1 & -1 & 1 \\ 1 & e^{ix_4} & e^{iy_4} \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 1 & -e^{ix_4} & -e^{iy_4} \end{bmatrix},$$

which has third row of form (5) or (7) respectively. By Example 3.7, this matrix is strongly balanced. Also, u_4 does not have form (10); otherwise

$$\begin{bmatrix} u_1 \\ u_3 \\ u_5 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & e^{ix_3} & e^{ix_3} \\ 1 & -1 & -1 \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 \\ 1 & e^{ix_3} & -1 \\ 1 & e^{iy_3} & -1 \end{bmatrix},$$

which has second and third row of form (C4), and the matrix is strongly balanced. Next, u_4 does not have form (12); otherwise the matrix with rows u_5, u_3, u_4 is equivalent to

$$\begin{bmatrix} u_5 \\ u_3 \\ u_4 \end{bmatrix} = \begin{bmatrix} 1 & -1 & -1 \\ 1 & 1 & e^{iy_3} \\ 1 & -e^{iy_4} & e^{iy_4} \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & -e^{iy_3} \\ 1 & e^{iy_4} & -e^{iy_4} \end{bmatrix}$$

where $y_3, y_4 \in \mathcal{P}$. This matrix has second row of form (C8) and third row of form (11), and hence is strongly balanced. Note that u_4 does not have form (C3); otherwise the

$$\begin{bmatrix} u_2 \\ u_3 \\ u_4 \end{bmatrix} = \begin{bmatrix} 1 & -1 & 1 \\ 1 & 1 & e^{iy_3} \\ 1 & e^{ix_4} & -1 \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & e^{iy_3} \\ 1 & -e^{ix_4} & -1 \end{bmatrix}$$

where $x_3, y_4 \in \mathcal{P}$. But then the second row has form (C7) and the third row has form (C4), and the matrix is strongly balanced. If u_4 has form (C6), then the matrix with rows u_1, u_3, u_4 is equivalent to

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & e^{iy_3} \\ 1 & 1 & e^{iy_4} \end{bmatrix}$$

and we are back to Case 1. Likewise, if u_4 has form (C7) or (C8), then

$$\begin{bmatrix} u_2 \\ u_4 \\ u_5 \end{bmatrix} = \begin{bmatrix} 1 & -1 & 1 \\ 1 & -1 & e^{iy_4} \\ 1 & -1 & -1 \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & e^{iy_4} \\ 1 & 1 & -1 \end{bmatrix}$$

and we are back to Case 1.

B. Assume u_4 and u_5 have neither form (C10) nor (C12). Recall from the beginning of this subsection that u_3 has form (2), (9) or (C5). Also, for $j = 4, 5$, u_j has form (2), (3), (6), (8) – (12), (C3), (C4), (C6), (C7) or (C8).

B.i. Suppose $\{e^{ix_3}, e^{ix_4}, e^{ix_5}\} \cap \{\pm 1\} = \emptyset$. Suppose u_3 has the form (2). Since the matrix with rows u_1, u_3, u_j is not strongly balanced for $j = 4, 5$, u_j has form (8) or (12) by Table 3.2. Since the matrix with rows u_1, u_4, u_5 is not strongly balanced, by Table 3.2, u_4 and u_5 do not have the same form. We may assume that u_4 has form (8) and u_5 has form (12), but then the matrix with rows u_1, u_4, u_5 is strongly balanced.

Suppose u_3 has form (9). Since the matrix with rows u_1, u_3, u_j is not strongly balanced for $j = 4, 5$, u_j has form (6), (8), (10), (11), (12) or (C3) by Table 3.2. However, note that u_3 has form (9) means that v_3 has form (12); since the matrix with rows v_1, v_3, v_j is not strongly balanced for $j = 4, 5$, by Table 3.2 v_j has form (2), (6), (9), (10), (11) or (C3). Accordingly, u_j can only have form (8), (10), (11) or (12). If u_j has form (8), then v_j has form (2) and we are back to Case A.i. If u_j has form (10), then we are back to Case 1 because

$$\begin{bmatrix} u_1 \\ u_3 \\ u_j \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & e^{ix_3} & e^{ix_3} \\ 1 & e^{ix_j} & e^{ix_j} \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 \\ e^{-ix_3} & 1 & 1 \\ e^{-ix_j} & 1 & 1 \end{bmatrix}$$

Now, u_j must have the from (11) or (12). As before, u_4 and u_5 cannot have the same form. We may assume that u_4 has form (11) and u_5 has form (12). But then

$$\begin{bmatrix} u_2 \\ u_4 \\ u_5 \end{bmatrix} = \begin{bmatrix} 1 & -1 & 1 \\ 1 & -e^{ix_4} & e^{ix_4} \\ 1 & -e^{ix_5} & e^{ix_5} \end{bmatrix} \sim \begin{bmatrix} 1 & e^{-ix_4} & e^{-ix_5} \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix},$$

and we are back to Case 1.

Finally, note that u_3 cannot have form (C5) because $e^{ix_3} \notin \{\pm 1\}$.

B.ii. Suppose $\{e^{ix_3}, e^{ix_4}, e^{ix_5}\} \cap \{\pm 1\} \neq \emptyset$. Suppose u_3 has form (2) or (9). Then there exists $j \in \{4, 5\}$ such that $e^{ix_j} = \pm 1$ while $e^{iy_j} \neq \pm 1$. Now, interchange rows 3 and j and if $e^{ix_j} = -1$, multiply the second column by -1 and interchange the first two rows. We may assume $y_3 \in \mathcal{P}$ since $A \sim \overline{A}$. Note that this new third row has form (C5). Therefore, we may assume that u_3 has form (C5). Recall that $e^{ix_j} \neq 1$ for $j = 4, 5$, else

$$\begin{bmatrix} u_1 \\ u_3 \\ u_j \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & e^{iy_3} \\ 1 & 1 & e^{iy_j} \end{bmatrix}$$

which is equivalent to a matrix of form (a) and we are back to Case 1. In other words, u_j does not have form (C6). Furthermore, by Table 3.2, u_j does not have form (2), (3), (9), (11), (C4) or (C5) else the matrix with rows u_1, u_3 and u_j is strongly balanced. In other words, u_j can only have one of the following forms: (6), (8), (10), (12), (C3), (C7) or (C8). But v_3 has form (C7) and hence, because the matrix with rows v_2, v_3 and v_j is not strongly balanced, therefore v_j has form (2), (11), (9), (C5) or (C6), i.e. u_j has form (8), (10), (12), (C7) or (C8).

Let $\{j,k\} = \{4,5\}$. Suppose u_j has form (8). Then u_k does not have form (8), (12) or (C7) else the matrix with rows u_1, u_j, u_k is strongly balanced. Note that v_j has form (2). If u_k has form (10) or (C8), then v_k has form (11) or (C6) and so the matrix with rows v_1, v_j and v_k is strongly balanced. Therefore, u_j cannot have form (8). Now suppose u_j has form (C7). But then the matrix with rows u_1, u_j and u_k] is strongly balanced for u_k of any form but (C8). However, if u_k has form (C8), then the matrix formed by rows u_2, u_j, u_k is equivalent to

$$\begin{bmatrix} u_2 \\ u_j \\ u_k \end{bmatrix} = \begin{bmatrix} 1 & -1 & 1 \\ 1 & -1 & e^{iy_j} \\ 1 & -1 & e^{iy_k} \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & e^{iy_j} & e^{iy_k} \end{bmatrix}$$

and we are back to Case 1.

We can now assume that u_j and u_k will have one of the following forms: (10), (12) or (C8). They will not have the same form, else the matrix with rows u_1, u_j and u_k will be strongly balanced. We will examine the restrictions on the entries in each of the possible combinations of forms by considering the following subcases.

B.ii.a. Suppose u_4 and u_5 have forms (C8) and (10) respectively. In other words, there exist $\alpha, \beta, \gamma \in \mathcal{P}$ such that

$$u_3 = [\ 1 \ \ 1 \ \ e^{i\alpha}\ ], \qquad u_4 = [\ 1 \ \ -1 \ \ e^{i(\beta-\pi)}\ ], \qquad u_5 = [\ 1 \ \ e^{i(\gamma-\pi)} \ \ e^{i(\gamma-\pi)}\ ].$$

By Table 3, we find conditions on these angles such that there are no 3×3 submatrices that can be strongly balanced. Because the matrix with rows u_1, u_4, u_5 is not strongly balanced,

$$\gamma \leq \beta. \tag{3.4.2}$$

Because the matrix with rows v_1, v_4, v_5 is not strongly balanced,

$$\gamma \geq \beta. \tag{3.4.3}$$

Equations (3.4.2) and (3.4.3) imply $\gamma = \beta$. Also, because the matrix with rows u_1, u_3, u_4 is not strongly balanced,

$$\gamma = \beta \leq \alpha. \tag{3.4.4}$$

Suppose $\gamma = \beta < \alpha$. For $j = 3, 4, 5$, let $\hat{u}_j$ be such that

$$\begin{bmatrix} u_3 \\ u_4 \\ u_5 \end{bmatrix} = \begin{bmatrix} 1 & 1 & e^{i\alpha} \\ 1 & -1 & e^{i(\beta-\pi)} \\ 1 & e^{i(\beta-\pi)} & e^{i(\beta-\pi)} \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & e^{i(\beta-\alpha-\pi)} \\ 1 & e^{i(\beta-\pi)} & e^{i(\beta-\alpha-\pi)} \end{bmatrix} = \begin{bmatrix} \hat{u}_3 \\ \hat{u}_4 \\ \hat{u}_5 \end{bmatrix}.$$

But $0 < \beta < \beta + (\pi - \alpha) < \alpha + (\pi - \alpha) = \pi$ and $e^{i(\beta+\pi-\alpha)} = e^{i(\beta-\alpha-\pi)}$. So $\hat{u}_4$ has form (C7) and $\hat{u}_5$ has form (8), and hence the matrix with rows $\hat{u}_3, \hat{u}_4, \hat{u}_5$ is strongly balanced. Therefore

$$\gamma = \beta = \alpha. \tag{3.4.5}$$

B.ii.b. Assume u_4 and u_5 have forms (C8) and (12) respectively. In other words, there exist $\alpha, \beta, \gamma \in \mathcal{P}$ such that

$$u_3 = \begin{bmatrix} 1 & 1 & e^{i\alpha} \end{bmatrix}, \qquad u_4 = \begin{bmatrix} 1 & -1 & e^{i(\beta-\pi)} \end{bmatrix}, \qquad u_5 = \begin{bmatrix} 1 & -e^{i\gamma} & e^{i\gamma} \end{bmatrix}.$$

But the matrix formed by rows $u_1, \ldots, u_5$ is equivalent, by complex conjugation, $(1,-1)$-signings and row permutation, to

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & e^{i\alpha} \\ 1 & -1 & e^{i(\beta-\pi)} \\ 1 & -e^{i\gamma} & e^{i\gamma} \end{bmatrix} \sim \begin{bmatrix} 1 & -1 & 1 \\ 1 & 1 & 1 \\ 1 & -1 & e^{-i\alpha} \\ 1 & 1 & e^{-i(\beta-\pi)} \\ 1 & e^{-i\gamma} & e^{-i\gamma} \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & e^{i(\pi-\beta)} \\ 1 & -1 & e^{-i\alpha)} \\ 1 & e^{-i\gamma} & e^{-i\gamma} \end{bmatrix}.$$

Note that the third, fourth and fifth rows of this matrix have forms (C5), (C8) and (10) respectively. Thus, by Case B.ii.a., $\alpha = \beta = \gamma$.

B.ii.c. Assume u_4 and u_5 have forms (10) and (12) respectively. Therefore, there exists $\alpha, \beta, \gamma \in \mathcal{P}$ such that

$$u_3 = [\ 1 \ \ 1 \ \ e^{i\alpha}\ ], \qquad u_4 = [\ 1 \ \ e^{i(\beta-\pi)} \ \ e^{i\beta}\ ], \qquad u_5 = [\ 1 \ \ e^{i(\gamma-\pi)} \ \ e^{i(\gamma-\pi)}\ ].$$

Once again, we use Table 3 to find necessary conditions on these angles for there to be no 3×3 submatrix that can be strongly balanced. Because the matrix with rows u_1, u_3, u_4 is not strongly balanced,

$$\beta \leq \alpha. \tag{3.4.6}$$

Because the matrix with rows v_1, v_3, v_4 is not strongly balanced,

$$\beta \geq \alpha. \tag{3.4.7}$$

Therefore, $\beta = \alpha$. Also, because the matrix with rows u_1, u_4, u_5 is not strongly balanced,

$$\gamma \leq \beta = \alpha. \tag{3.4.8}$$

Suppose $\gamma < \beta = \alpha$. For $j = 3, 4, 5$, let $\hat{u}_j$ be such that

$$\begin{bmatrix} u_3 \\ u_4 \\ u_5 \end{bmatrix} = \begin{bmatrix} 1 & 1 & e^{i\alpha} \\ 1 & e^{i(\alpha-\pi)} & e^{i\alpha} \\ 1 & e^{i(\gamma-\pi)} & e^{i(\gamma-\pi)} \end{bmatrix} \sim \begin{bmatrix} 1 & e^{i(\pi-\gamma)} & e^{i(\alpha+\pi-\gamma)} \\ 1 & e^{i(\alpha-\gamma)} & e^{i(\alpha+\pi-\gamma)} \\ 1 & 1 & 1 \end{bmatrix} \sim \begin{bmatrix} \hat{u}_3 \\ \hat{u}_4 \\ \hat{u}_5 \end{bmatrix}.$$

Because $\gamma < \alpha$, thus $0 < (\alpha - \gamma) < \pi - \gamma < \pi$. Also, $e^{i(\alpha-\gamma+\pi)} = e^{i(\alpha-\gamma-\pi)}$. So $\hat{u}_4$ has form (11) and $\hat{u}_3$ has form (6), and therefore the matrix with rows $\hat{u}_5, \hat{u}_3, \hat{u}_4$ is strongly balanced. Hence

$$\gamma = \beta = \alpha. \tag{3.4.9}$$

Now that we know some conditions on rows u_4 and u_5, we consider the 5×5 matrix and see what values other entries must have. First, for $\alpha \in \mathcal{P}$, let

$$A_1 = \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & e^{i\alpha} \end{bmatrix}, \quad b_1 = \begin{bmatrix} 1 & -1 & -e^{i\alpha} \end{bmatrix},$$

$$b_2 = \begin{bmatrix} 1 & -e^{i\alpha} & -e^{i\alpha} \end{bmatrix}, \quad b_3 = \begin{bmatrix} 1 & -e^{i\alpha} & e^{i\alpha} \end{bmatrix}.$$

Note that because $A_1^t = A_1$,

$$A = \begin{bmatrix} A_1 & v_4^t & v_5^t \\ u_4 & e^{iz_{44}} & e^{iz_{45}} \\ u_5 & e^{iz_{54}} & e^{iz_{55}} \end{bmatrix},$$

where $u_4, u_5, v_4, v_5 \in \{b_1, b_2, b_3\}$. First, we use the 4×4 submatrices

$$\begin{bmatrix} A_1 & v_j^t \\ u_k & e^{iz_{kj}} \end{bmatrix}$$

to show that $e^{iz_{kj}} \in \{\pm 1, \pm e^{i\alpha}\}$ and that $e^{i\alpha} = i$. (Recall that $\alpha \in \mathcal{P}$).

Suppose $v_j = b_1$. Note that

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & e^{i\alpha} & -e^{i\alpha} \\ 1 & r & s & t \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 & 1 \\ -1 & 1 & -1 & 1 \\ 1 & 1 & e^{i\alpha} & -e^{i\alpha} \\ \bar{r} & 1 & \bar{r}s & \bar{r}t \end{bmatrix}$$

$$\sim \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -e^{i\alpha} & e^{i\alpha} \\ 1 & \bar{r} & \bar{r}t & \bar{r}s \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -e^{-i\alpha} & e^{-i\alpha} \\ 1 & r & r\bar{t} & r\bar{s} \end{bmatrix}.$$

Therefore, $r, r\bar{t} \in \{\pm 1, \pm e^{-i\alpha}\}$. Let $u_k = [1, r, s]$ and $e^{iz_{kj}} = t$. Note that if $u_k \in \{b_2, b_3\}$, then $r = -e^{i\alpha}$. But this implies $-e^{i\alpha} = e^{-i\alpha}$, i.e. $e^{i\alpha} = i$. And thus $t \in \{\pm 1, \pm i\}$. If $u_k = b_1$, then $r = -1$ and $t \in \{\pm 1, \pm e^{i\alpha}\}$.

Suppose $v_j = b_2$. Note that

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -e^{i\alpha} \\ 1 & 1 & e^{i\alpha} & -e^{i\alpha} \\ 1 & r & s & t \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & e^{-i\alpha} & -e^{-i\alpha} \\ 1 & -1 & e^{-i\alpha} & 1 \\ 1 & 1 & 1 & 1 \\ 1 & r & se^{-i\alpha} & -te^{-i\alpha} \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & e^{-i\alpha} \\ 1 & 1 & -e^{-i\alpha} & e^{-i\alpha} \\ 1 & r & -te^{-i\alpha} & se^{-i\alpha} \end{bmatrix}.$$

Therefore, $r, -te^{-i\alpha} \in \{\pm 1, \pm e^{-i\alpha}\}$. Let $u_k = [1, r, s]$ and $e^{iz_{kj}} = t$. Note that if $u_k \in \{b_2, b_3\}$, then $r = -e^{i\alpha}$. But then $-e^{i\alpha} = e^{-i\alpha}$, i.e. $e^{i\alpha} = i$. And thus $t \in \{\pm 1, \pm i\}$. If $u_k = b_1$, then $r = -1$ and $t \in \{\pm 1, \pm e^{i\alpha}\}$.

Now suppose $v_j = b_3$. Note that

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -e^{i\alpha} \\ 1 & 1 & e^{i\alpha} & e^{i\alpha} \\ 1 & r & s & t \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 & 1 \\ -1 & 1 & -1 & e^{i\alpha} \\ 1 & 1 & e^{i\alpha} & e^{i\alpha} \\ \overline{r} & 1 & s\overline{r} & t\overline{r} \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & e^{-i\alpha} & e^{-i\alpha}1 \\ -1 & 1 & -e^{-i\alpha} & 1 \\ 1 & 1 & 1 & 1 \\ \overline{r} & 1 & s\overline{r}e^{-i\alpha} & t\overline{r}e^{-i\alpha} \end{bmatrix}$$

$$\sim \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -e^{-i\alpha} \\ 1 & 1 & e^{-i\alpha} & e^{-i\alpha} \\ 1 & \overline{r} & t\overline{r}e^{-i\alpha} & s\overline{r}e^{-i\alpha} \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -e^{i\alpha} \\ 1 & 1 & e^{i\alpha} & e^{i\alpha} \\ 1 & r & r\overline{t}e^{i\alpha} & r\overline{s}e^{i\alpha} \end{bmatrix}.$$

So $r, r\overline{t}e^{i\alpha} \in \{\pm 1, \pm e^{i\alpha}\}$, i.e. $t \in \{\pm r, \pm re^{i\alpha}\}$. Let $u_k = [1, r, s]$. If $u_k = b_1$ then $r = -1$ and so $e^{iz_{kj}} = t \in \{\pm 1, \pm e^{i\alpha}\}$. If $u_k \in \{b_2, b_3\}$, or in other words, $r = -e^{i\alpha}$, then $t \in \{\pm e^{i\alpha}, \pm e^{i2\alpha}\}$.

Note that there are 3 choices for the two vectors v_j, therefore, at least one, say v_4 is in $\{b_1, b_2\}$. Similarly, there are two vectors u_k, thus at least one of them, say u_4 is in $\{b_2, b_3\}$. Therefore, $e^{i\alpha} = i$, and so $e^{i2\alpha} = -1$ and $e^{iz_{kj}} \in \{\pm 1, \pm i\}$ for all $j, k = 4, 5$. By Lemma 3.3 (a), A is not ray-nonsingular.

3.4.3 Case 3

Assume that the leading 3×3 principal submatrix of A has form (c) and that A is not equivalent to a matrix B whose principal submatrix has form (a), (b) or is strongly balanced. Let

$$\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & e^{i\alpha} \\ 1 & e^{i\beta} & -1 \\ 1 & e^{ix_4} & e^{iy_4} \\ 1 & e^{ix_5} & e^{iy_5} \end{bmatrix}.$$

We may assume that $e^{i\alpha}, e^{i\beta} \neq \pm 1$; otherwise, we are back to Case 1 or Case 2. Furthermore, we may assume that $\alpha \in \mathcal{P}$ as $A \sim \overline{A}$. Therefore, u_2 has form (C7). Since the matrix with rows u_1, u_2 and u_3 is not strongly balanced, by Table 3.2, u_3 has form (C3), i.e. $\beta \in \mathcal{P}$. Also, note that $e^{ix_j}, e^{iy_j} \neq \pm 1$ for $j = 4, 5$; otherwise, there exists a submatrix of the form (a) or (b). For $j = 4, 5$, since the matrix with rows u_1, u_3 and u_j is not strongly balanced, u_j has form (1), (7), (8), (9) or (12) by Table 3.2. Since the matrix with rows u_1, u_2 and u_j is also not strongly balanced, u_j can only have form (9). But this means that rows u_4 and u_5 both have form (9) and therefore the matrix with rows u_1, u_4 and u_5 is strongly balanced, which is the desired contradiction.

3.4.4 Case 4

Assume that the leading 3×3 principal submatrix of A has form (d) and that A is not equivalent to a matrix B whose principal submatrix has form (a), (b), (c) or is strongly balanced. First, let

$$\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & e^{i\alpha} \\ 1 & e^{i\beta} & -1 \\ 1 & e^{ix_4} & e^{iy_4} \\ 1 & e^{ix_5} & e^{iy_5} \end{bmatrix}.$$

We may assume that $e^{i\alpha}, e^{i\beta} \neq \pm 1$; otherwise, we are back to Case 1 or Case 2. Furthermore, we may assume that $\alpha \in \mathcal{P}$ as $A \sim \overline{A}$. Therefore, u_2 has form (C5). Since the matrix with rows u_1, u_2 and u_3 is not strongly balanced, by Table 3.2, u_3 has form (C3), i.e. $\beta \in \mathcal{P}$. Also, note that $e^{ix_j}, e^{iy_j} \neq \pm 1$ for $j = 4, 5$, else there exists a submatrix of the form (a) or (b). As in Case 3 in the previous subsection, u_3 has form (C3), and so for $j = 4, 5$, u_j has form (1), (7), (8), (9) or (12). Since the matrix with rows u_1, u_2 and u_j is also not strongly balanced, u_j can only have form (1), (8) or (12). By Table 3.2, we see that the pairwise intersections of the solution sets are non-empty; thus, the matrix with rows u_1, u_4 and u_5 is strongly balanced.

3.4.5 Case 5

Assume that the leading 3×3 principal submatrix of A has form (e) and that A is not equivalent to a matrix B whose principal submatrix has form (a), (b), (c), (d) or is strongly balanced. We will show that this implies that $a_{ij} \in \{1, e^{\pm i2\pi/3}\}$ and that A has a 4×4 strongly balanced submatrix.

Suppose $u_1, \ldots, u_5$ are the five rows of $[a_{ij}]_{1\le i\le 5, 1\le j\le 3}$. Then

$$\begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & e^{i\beta} \\ 1 & e^{i\alpha} & 1 \end{bmatrix}.$$

Let

$$u_4 = [\ 1 \quad e^{ix_4} \quad e^{iy_4}\ ], \quad u_5 = [\ 1 \quad e^{ix_5} \quad e^{iy_5}\ ].$$

Note that $e^{i\alpha}, e^{i\beta}, e^{ix_j}, e^{iy_j} \neq \pm 1$, for $j = 4, 5$; otherwise we are back to Case 1 or Case 2. Furthermore, we may assume that $\alpha \in \mathcal{P}$, otherwise replace A with $\overline{A}$. Therefore, u_3 has form (C1). Because the matrix with row u_1, u_2, u_3 is not strongly balanced, by Table 2, u_2 has form (C5), i.e. $\beta \in \mathcal{P}$. We also know that

$$\pi \le \alpha + \beta \tag{3.4.10}$$

by Table 3. Because the matrix with rows u_1, u_2, u_j, for $j = 4, 5$, is not strongly balanced, u_j has forms (1), (4), (6), (8), (10) or (12). Because the matrix with rows u_1, u_3, u_j is also not strongly balanced, u_j has one of the following forms:

(6), (8) or (10).

We now consider the three cases where u_j has form (6), (8) and (10) and examine the matrices with rows u_l, u_k, u_j where $l, k \in \{1, 2, 3\}$, to find bounds on x_j and y_j dependent on α and β. These bounds are found by using Table 3 for the given matrices.

A. Suppose u_j has form (6), i.e., $x_j \in \mathcal{P}$, $y_j \in \mathcal{N}$ and $x_j - y_j > \pi$. Because the matrix with rows u_1, u_2, u_j is not strongly balanced,

$$0 < y_j - \beta + 2\pi \leq x_j. \tag{3.4.11}$$

Because the matrix with rows u_1, u_3, u_j is not strongly balanced,

$$x_j \leq \alpha. \tag{3.4.12}$$

Note that the following matrices are equivalent.

$$\begin{bmatrix} u_2 \\ u_3 \\ u_j \end{bmatrix} = \begin{bmatrix} 1 & 1 & e^{i\beta} \\ 1 & e^{i\alpha} & 1 \\ 1 & e^{ix_j} & e^{iy_j} \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 \\ 1 & e^{i\alpha} & e^{-i\beta} \\ 1 & e^{ix_j} & e^{i(y_j-\beta)} \end{bmatrix}.$$

The second row of the second matrix has form (6) or (11) because $a + \beta \geq \pi$ by (3.4.10). Because $e^{i(y_j-\alpha)} = e^{i(y_j-\alpha+2\pi)}$ and (3.4.11) holds, the third column has either form (1) or (9). By Table 3,

$$\alpha \leq x_j. \tag{3.4.13}$$

Equations (3.4.12) and (3.4.13) imply

$$\alpha = x_j. \tag{3.4.14}$$

Also, equation (3.4.11) implies

$$\alpha + \beta \geq y_j + 2\pi > \pi. \tag{3.4.15}$$

B. Assume u_j has form (8), i.e., $x_j \in \mathcal{N}$, $y_j \in \mathcal{P}$ and $y_j - x_j > \pi$. Note that the following matrices are equivalent.

$$\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & e^{i\beta} \\ 1 & e^{i\alpha} & 1 \\ 1 & e^{ix_j} & e^{iy_j} \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & e^{i\alpha} \\ 1 & e^{i\beta} & 1 \\ 1 & e^{iy_j} & e^{ix_j} \end{bmatrix}.$$

Using the same argument in Case A, we have

$$y_j = \beta \text{ and} \tag{3.4.16}$$

$$\alpha + \beta \geq x_j + 2\pi > \pi. \tag{3.4.17}$$

C. Assume u_j has form (10), i.e. $x_j = y_j \in \mathcal{N}$. Because the matrix with rows u_1, u_2, u_j is not strongly balanced,

$$\beta \geq x_j + \pi. \tag{3.4.18}$$

Also, because the matrix with rows u_1, u_3, u_j is not strongly balanced,

$$\alpha \geq x_j + \pi. \tag{3.4.19}$$

We now use the above information to further determine the structure of $u_1, \ldots, u_5$. We have the following three cases.

A$'$. Assume u_4 and u_5 have forms (6) and (8) respectively. Then $x_4 = \alpha$, $y_5 = \beta$ and $\alpha + \beta \geq \gamma + 2\pi > \pi$ where $\gamma = y_4$ and x_5. Suppose that $\alpha + \beta > y_4 + 2\pi$. Then the following matrices are equivalent.

$$\begin{bmatrix} u_2 \\ u_4 \\ u_5 \end{bmatrix} = \begin{bmatrix} 1 & 1 & e^{i\beta} \\ 1 & e^{i\alpha} & e^{iy_4} \\ 1 & e^{ix_5} & e^{i\beta} \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 \\ 1 & e^{i\alpha} & e^{i(y_4-\beta)} \\ 1 & e^{ix_5} & 1 \end{bmatrix}.$$

But the second row has form (1) and the third row has form (C2) and, by Table 3.2, the matrix is strongly balanced. Therefore,

$$\alpha + \beta = y_4 + 2\pi. \tag{3.4.20}$$

Similarly, using the matrix with rows u_3, u_4, u_5, we can show that

$$\alpha + \beta = x_5 + 2\pi. \tag{3.4.21}$$

Therefore,

$$\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & e^{i\beta} \\ 1 & e^{i\alpha} & 1 \\ 1 & e^{i\alpha} & e^{i(\alpha+\beta)} \\ 1 & e^{i(\alpha+\beta)} & e^{i\beta} \end{bmatrix}.$$

B′. Assume u_4 and u_5 have forms (6) and (10) respectively. Then

$$x_4 = \alpha, \qquad \alpha + \beta \geq y_4 + 2\pi > \pi,$$

$$x_5 = y_5 \in \mathcal{N} \qquad \text{and } x_5 + \pi \leq \alpha, \beta.$$

Because the matrix with rows u_1, u_4, u_5 is not strongly balanced,

$$y_4 \geq x_5. \tag{3.4.22}$$

Note that

$$\begin{bmatrix} u_2 \\ u_4 \\ u_5 \end{bmatrix} = \begin{bmatrix} 1 & 1 & e^{i\beta} \\ 1 & e^{i\alpha} & e^{iy_4} \\ 1 & e^{ix_5} & e^{ix_5} \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 \\ 1 & e^{i\alpha} & e^{i(y_4-\beta)} \\ 1 & e^{ix_5} & e^{i(x_5-\beta)} \end{bmatrix}.$$

Label the second row $\hat{u}_4$ and the third row $\hat{u}_5$. By equation (3.4.15), we know $\hat{u}_4$ has form (1) if $y_4 2\pi < \alpha+\beta$ or (9) if $y_4+2\pi = \alpha+\beta$. Also, by (3.4.18) and $x_5-\alpha > x_5-\pi$, we see that $\hat{u}_5$ has form (8) if $\beta > x_5+\pi$ or (C4) if $\beta = x_5+\pi$. Referring to Table 3.2, we see that $\hat{u}_4$ must have form (9), i.e. $y_4 2\pi = \alpha+\beta$, and $\hat{u}_5$ must have form (8), i.e. $\beta > x_5+\pi$ because this matrix is not strongly balanced.

Similarly, we note that the matrix

$$\begin{bmatrix} u_3 \\ u_4 \\ u_5 \end{bmatrix} = \begin{bmatrix} 1 & e^{i\alpha} & 1 \\ 1 & e^{i\alpha} & e^{iy_4} \\ 1 & e^{ix_5} & e^{ix_5} \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & e^{iy_4} \\ 1 & e^{i(x_5-\alpha)} & e^{ix_5} \end{bmatrix}.$$

Again, label the second row $\hat{u}_4$ and the third row $\hat{u}_5$. Note that $\hat{u}_4$ has form (C6) and $\hat{u}_5$ has form (6) or (C8) because $x_5-\alpha > x_5-\pi$ and (3.4.19). But this matrix is not strongly balanced and so by Table 3,

$$x_5 \geq y_4. \tag{3.4.23}$$

Equations (3.4.22), (3.4.23) and the refinement of (3.4.15) imply

$$x_5 = y_4 = \alpha+\beta-2\pi. \tag{3.4.24}$$

So

$$\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & e^{i\beta} \\ 1 & e^{i\alpha} & 1 \\ 1 & e^{i\alpha} & e^{i(\alpha+\beta)} \\ 1 & e^{i(\alpha+\beta)} & e^{i(\alpha+\beta)} \end{bmatrix}.$$

C$'$. Assume u_4 and u_5 have forms (8) and (10) respectively. Then

$$\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & e^{i\beta} \\ 1 & e^{i\alpha} & 1 \\ 1 & e^{ix_4} & e^{i\beta} \\ 1 & e^{ix_5} & e^{ix_5} \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & e^{i\alpha} \\ 1 & e^{i\beta} & 1 \\ 1 & e^{i\beta} & e^{ix_4} \\ 1 & e^{ix_5} & e^{ix_5} \end{bmatrix}.$$

Using the argument in Case B$'$, we see that

$$x_5 = x_4 = \alpha + \beta - 2\pi$$

and

$$\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & e^{i\beta} \\ 1 & e^{i\alpha} & 1 \\ 1 & e^{i(\alpha+\beta)} & e^{i\beta} \\ 1 & e^{i(\alpha+\beta)} & e^{i(\alpha+\beta)} \end{bmatrix}.$$

Let

$$c_1 = \begin{bmatrix} 1 & e^{i\alpha} & e^{i(\alpha+\beta)} \end{bmatrix}, \quad c_2 = \begin{bmatrix} 1 & e^{i(\alpha+\beta)} & e^{i\beta} \end{bmatrix}, \quad c_3 = \begin{bmatrix} 1 & e^{i(\alpha+\beta)} & e^{i(\alpha+\beta)} \end{bmatrix},$$

$$c_4 = \begin{bmatrix} 1 & e^{i\beta} & e^{i(\alpha+\beta)} \end{bmatrix}, \quad c_5 = \begin{bmatrix} 1 & e^{i(\alpha+\beta)} & e^{i\alpha} \end{bmatrix}.$$

Using both A by A^t, we see that if A_1 is the 3×3 leading principal submatrix of A, i.e., with rows u_1, u_2, u_3, then

$$A = \begin{bmatrix} A_1 & v_4^t & v_5^t \\ u_4 & e^{iz_{44}} & e^{iz_{45}} \\ u_5 & e^{iz_{54}} & e^{iz_{55}} \end{bmatrix}$$

where $u_4, u_5 \in \{c_1, c_2, c_3\}$ and $v_4, v_5 \in \{c_3, c_4, c_5\}$. We consider the possible 4×4 submatrices for the different values of u_j and v_k and determine the possible values of $e^{iz_{kj}}$.

Suppose $u_j = c_3$. Let $v_k = [1, e^{i\gamma}, e^{i\delta}]$ and $z_{kj} = \lambda$. We consider the following submatrix of A^t:

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & e^{i\alpha} & e^{i(\alpha+\beta)} \\ 1 & e^{i\beta} & 1 & e^{i(\alpha+\beta)} \\ 1 & e^{i\gamma} & e^{i\delta} & e^{i\lambda} \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & e^{-i\alpha} & e^{-i(\alpha+\beta)} \\ 1 & 1 & 1 & 1 \\ 1 & e^{i\beta} & e^{-i\alpha} & 1 \\ 1 & e^{i\gamma} & e^{i(\delta-\alpha)} & e^{i(\lambda-\alpha-\beta)} \end{bmatrix}$$

$$\sim \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & e^{-i(\alpha+\beta)} & e^{-i\alpha} \\ 1 & e^{i\beta} & 1 & e^{-i\alpha} \\ 1 & e^{i\gamma} & e^{i(\lambda-\alpha-\beta)} & e^{i(\delta-\alpha)} \end{bmatrix}.$$

Applying the arguments in Cases A, B, C, A′, B′, C′ to the right most matrix with

(α, β) replaced by $(\beta, -(\alpha+\beta))$, we conclude that

$$\begin{bmatrix} 1 \\ e^{i\gamma} \\ e^{i(\lambda-\alpha-\beta)} \end{bmatrix} \in \left\{ \begin{bmatrix} 1 \\ e^{i\beta} \\ e^{-i\alpha} \end{bmatrix}, \begin{bmatrix} 1 \\ e^{-i\alpha} \\ e^{-i(\alpha+\beta)} \end{bmatrix}, \begin{bmatrix} 1 \\ e^{-i\alpha} \\ e^{-i\alpha} \end{bmatrix} \right\}.$$

Thus, $e^{i\lambda} \in \{1, e^{i\beta}\}$ and $e^{i\gamma} \in \{e^{i\beta}, e^{i(-\alpha)}\}$. Because $-\alpha, (\alpha+\beta) \in \mathcal{N}$ and $\beta \in \mathcal{P}$, if $v_k = c_3$ or c_5, then $e^{i\gamma} = e^{i(\alpha+\beta)} = e^{-i\alpha}$, i.e. $e^{i(2\alpha+\beta)} = 1$.

Now suppose $u_j = c_2$. Let $v_k = [1, e^{i\gamma}, e^{i\delta}]$ and $z_{kj} = \lambda$. We consider the following submatrix of A^t:

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & e^{i\alpha} & e^{i(\alpha+\beta)} \\ 1 & e^{i\beta} & 1 & e^{i\beta} \\ 1 & e^{i\gamma} & e^{i\delta} & e^{i\lambda} \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 & 1 \\ e^{-i\alpha} & e^{-i\alpha} & 1 & e^{i\beta} \\ 1 & e^{i\beta} & 1 & e^{i\beta} \\ e^{-i\delta} & e^{i(\gamma-\delta)} & 1 & e^{i(\lambda-\delta)} \end{bmatrix}$$

$$\sim \begin{bmatrix} 1 & e^{-i\beta} & 1 & e^{-i\beta} \\ e^{-i\alpha} & e^{-i(\beta+\alpha)} & 1 & 1 \\ 1 & 1 & 1 & 1 \\ e^{-i\delta} & e^{i(\gamma-\delta-\beta)} & 1 & e^{i(\lambda-\delta-\beta)} \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & e^{-i\beta} & e^{-i\beta} \\ 1 & e^{-i\alpha} & 1 & e^{-i(\alpha+\beta)} \\ 1 & e^{-i\delta} & e^{i(\lambda-\delta-\beta)} & e^{i(\gamma-\delta-\beta)} \end{bmatrix}.$$

Applying the arguments in Cases A, B, C, A′, B′, C′ to the right most matrix with (α, β) replaced by $(-\alpha, -\beta)$, we conclude that

$$\begin{bmatrix} 1 \\ e^{-i\delta} \\ e^{i(\lambda-\delta-\beta)} \end{bmatrix} \in \left\{ \begin{bmatrix} 1 \\ e^{-i\alpha} \\ e^{-i(\alpha+\beta)} \end{bmatrix}, \begin{bmatrix} 1 \\ e^{-i(\alpha+\beta)} \\ e^{-i\beta} \end{bmatrix}, \begin{bmatrix} 1 \\ e^{-i(\alpha+\beta)} \\ e^{-i(\alpha+\beta)} \end{bmatrix} \right\}.$$

Thus, $e^{i\lambda} \in \{e^{i\delta}, e^{i(\delta-\alpha)}\}$. Also,

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & e^{i\alpha} & e^{i(\alpha+\beta)} \\ 1 & e^{i\beta} & 1 & e^{i\beta} \\ 1 & e^{i\gamma} & e^{i\delta} & e^{i\lambda} \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & e^{i\alpha} & e^{i(\alpha+\beta)} \\ e^{-i\beta} & 1 & e^{-i\beta} & 1 \\ e^{-i\gamma} & 1 & e^{i(\delta-\gamma)} & e^{i(\lambda-\gamma)} \end{bmatrix}$$

$$\sim \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & e^{i(\alpha+\beta)} & e^{i\alpha} \\ 1 & e^{-i\beta} & 1 & e^{-i\beta} \\ 1 & e^{-i\gamma} & e^{i(\lambda-\gamma)} & e^{i(\delta-\gamma)} \end{bmatrix}.$$

Applying the arguments in A, B, C, A′, B′, C′ to the right most matrix with (α, β) replaced by $(-\beta, \alpha+\beta)$, we conclude that

$$\begin{bmatrix} 1 \\ e^{-i\gamma} \\ e^{i(\lambda-\gamma)} \end{bmatrix} \in \left\{ \begin{bmatrix} 1 \\ e^{-i\beta} \\ e^{i\alpha} \end{bmatrix}, \begin{bmatrix} 1 \\ e^{i\alpha} \\ e^{i(\alpha+\beta)} \end{bmatrix}, \begin{bmatrix} 1 \\ e^{i\alpha} \\ e^{i\alpha} \end{bmatrix} \right\}.$$

Thus, $e^{i\lambda} \in \{e^{i(\alpha+\beta+\gamma)}, e^{i(\alpha+\gamma)}\}$ and $e^{i\gamma} \in \{e^{i(-\alpha)}, e^{i\beta}\}$. Since $-\alpha \in \mathcal{N}$ and $\beta \in \mathcal{P}$, if $v_k = c_3$ or c_5, then $e^{i\gamma} = e^{i(\alpha+\beta)} = e^{-i\alpha}$. In other words, $e^{i(2\alpha+\beta)} = 1$. Furthermore, if $v_k = c_3$, then $e^{i\delta} = e^{i(\alpha+\beta)}$ and therefore, $e^{i\lambda} \in \{e^{i(\alpha+\beta)}, e^{i\beta}\} \bigcap \{e^{i\beta}, 1\}$. So $e^{i\lambda} = e^{i\beta}$. If $v_k = c_5$, then $e^{i\delta} = e^{i\alpha}$; therefore, $e^{i\lambda} \in \{e^{i\alpha}, 1\} \bigcap \{e^{i\beta}, 1\}$. So either $e^{i\lambda} = 1$ or $e^{i\lambda} = e^{i\alpha} = e^{i\beta}$. If $v_k = c_4$, then $e^{i\delta} = e^{i(\alpha+\beta)}$ and $e^{i\gamma} = e^{i\beta}$. Hence, $e^{i\lambda} \in \{e^{i(\alpha+\beta)}, e^{i\beta}\} \bigcap \{e^{i(2\beta+\alpha)}, e^{i(\alpha+\beta)}\}$. Recall that $\alpha, \beta \in \mathcal{P} = (0, \pi)$. Thus, $e^{i\lambda} = e^{i(\alpha+\beta)}$.

Suppose $u_j = c_1$. Let $v_k = [1, e^{i\gamma}, e^{i\delta}]$ and $z_{kj} = \lambda$. We consider the following submatrix of A^t:

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & e^{i\alpha} & e^{i\alpha} \\ 1 & e^{i\beta} & 1 & e^{i(\alpha+\beta)} \\ 1 & e^{i\gamma} & e^{i\delta} & e^{i\lambda} \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & e^{i\beta} & e^{i(\alpha+\beta)} \\ 1 & e^{i\alpha} & 1 & e^{i\alpha} \\ 1 & e^{i\delta} & e^{i\gamma} & e^{i\lambda} \end{bmatrix}.$$

Interchanging the roles of (α, γ) and (β, δ), we see that this is similar to the case when $u_j = c_2$. In other words,

$$e^{i\lambda} \in \{e^{i\gamma}, e^{i(\gamma-\beta)}\} \bigcap \{e^{i(\alpha+\beta+\delta)}, e^{i(\beta+\gamma)}\} \text{ and } e^{i\delta} \in \{e^{i(-\beta)}, e^{i\alpha}\}.$$

If $v_k = c_3$ or c_4, then $e^{i\delta} = e^{i(\alpha+\beta)}$ and so $e^{i(\alpha+\beta)} = e^{-i\beta}$, i.e. $e^{i(2\beta+\alpha)} = 1$. Furthermore, if $v_k = c_3$, then $e^{i\lambda} = e^{i\alpha}$. If $v_k = c_4$, then either $e^{i\lambda} = 1$ or $e^{i\lambda} = e^{i\alpha} = e^{i\beta}$. If $v_k = c_5$, then $e^{i\lambda} = e^{i(\alpha+\beta)}$.

Now suppose that $v_j = c_5$. Let $u_k = [1, e^{i\gamma}, e^{i\delta}]$ and $z_{jk} = \lambda$. Interchanging α and β, and using the transpose of A, we see that this is similar to the case when $u_j = c_2$. Thus, $e^{i\lambda} \in \{e^{i\delta}, e^{i(\delta-\beta)}\} \bigcap \{e^{i(\alpha+\beta+\gamma)}, e^{i(\beta+\gamma)}\}$ and $e^{i\gamma} \in \{e^{i\alpha}, e^{-i\beta}\}$. Therefore, if $u_k = c_2$ or c_3, then $e^{i\gamma} = e^{i(\alpha+\beta)} = e^{-i\beta}$, i.e. $e^{i(\alpha+2\beta)} = 1$. Furthermore, if $u_k = c_3$, then $e^{i\lambda} = e^{i\alpha}$. If $u_k = c_2$, then either $e^{i\lambda} = 1$ or $e^{i\lambda} = e^{i\beta} = e^{i\alpha}$. And if $u_k = c_1$, then $e^{i\lambda} = e^{i(\alpha+\beta)}$.

Suppose that $v_j = c_4$. Let $u_k = [1, e^{i\gamma}, e^{i\delta}]$ and $z_{jk} = \lambda$. Interchanging α and β, and using the transpose of A, we see that this is similar to the case when $u_j = c_1$. Hence, $e^{i\lambda} \in \{e^{i\gamma}, e^{i(\gamma-\alpha)}\} \bigcap \{e^{i(\alpha+\beta+\delta)}, e^{i(\alpha+\delta)}\}$ and $e^{i\delta} \in \{e^{i\beta}, e^{-i\alpha}\}$. Therefore, if $u_k = c_1$ or c_3, then $e^{i\delta} = e^{i(\alpha+\beta)} = e^{-i\alpha}$, i.e. $e^{i(2\alpha+\beta)} = 1$. Furthermore, if $u_k = c_3$, then $e^{i\lambda} = e^{i\beta}$. And if $u_k = c_1$, then either $e^{i\lambda} = 1$ or $e^{i\lambda} = e^{i\beta} = e^{i\alpha}$. If $u_k = c_2$, then $e^{i\lambda} = e^{i(\alpha+\beta)}$.

Lastly, suppose $v_j = c_3$. Let $u_k = [1, e^{i\gamma}, e^{i\delta}]$ and $z_{jk} = \lambda$. Interchanging α and β, and using the transpose of A, we see that this is similar to the case when $u_j = c_3$. Thus, $e^{i\lambda} \in \{1, e^{i\alpha}\}$ and $e^{i\gamma} \in \{e^{i\alpha}, e^{-i\beta}\}$. So, if $u_k = c_2$ or c_3, then $e^{i\gamma} = e^{i(\alpha+\beta)} = e^{-i\beta}$. In other words, $e^{i(\alpha+2\beta)} = 1$.

Note that $\{u_4, u_5\} \bigcap \{c_2, c_3\} \neq \emptyset$ and also $\{v_4, v_5\} \bigcap \{c_3, c_5\} \neq \emptyset$. Therefore, $e^{-i\beta} = e^{i(\alpha+\beta)} = e^{-i\alpha}$ and so $\alpha = \beta$ and $e^{i(3\alpha)} = 1$. Let $\omega = e^{i\alpha}$ so that $w^2 = e^{i(\alpha+\beta)}$.

We can always assume that if $c_3 \in \{u_4, u_5, v_4, v_5\}$, then $u_5 = c_3$ (since $A \sim A^t$ and $A \sim PAQ$ where P, Q are permutation matrices). Also, if $u_j = c_1$, then interchange the second and third row and column to get $u_j = c_2$. Thus, we may assume that the pair of pairs $((u_4, u_5), (v_4, v_5))$ is one of the following: $((c_2, c_3), (c_5, c_3))$, $((c_2, c_3), (c_4, c_3))$, $((c_2, c_3), (c_5, c_4))$, $((c_2, c_1), (c_5, c_4))$. Hence, A is one of the following matrices:

$$B_1 = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & \omega & \omega^2 & \omega^2 \\ 1 & \omega & 1 & \omega & \omega^2 \\ 1 & \omega^2 & \omega & x_1 & \omega \\ 1 & \omega^2 & \omega^2 & \omega & y_1 \end{bmatrix}, \quad B_2 = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & \omega & \omega & \omega^2 \\ 1 & \omega & 1 & \omega^2 & \omega^2 \\ 1 & \omega^2 & \omega & \omega^2 & \omega \\ 1 & \omega^2 & \omega^2 & \omega & x_2 \end{bmatrix},$$

$$B_3 = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & \omega & \omega^2 & \omega \\ 1 & \omega & 1 & \omega & \omega^2 \\ 1 & \omega^2 & \omega & x_3 & \omega^2 \\ 1 & \omega^2 & \omega^2 & \omega & \omega \end{bmatrix}, \qquad B_4 = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & \omega & \omega^2 & \omega \\ 1 & \omega & 1 & \omega & \omega^2 \\ 1 & \omega^2 & \omega & x_4 & \omega^2 \\ 1 & \omega & \omega^2 & \omega^2 & y_4 \end{bmatrix},$$

with $x_i, y_i \in \{1, \omega\}$ for $i = 1, \ldots, 4$. However, if x_1, y_1, x_2, x_3 or $y_4 = \omega$, then we are back to Case 1 because A has the submatrix

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & \omega^2 & \omega \\ 1 & \omega^2 & \omega \end{bmatrix} \sim \begin{bmatrix} 1 & \omega & \omega^2 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}.$$

Also, if $x_4 = \omega$, then we are back to Case 1 because A has the submatrix

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & \omega & \omega^2 \\ 1 & \omega & \omega^2 \end{bmatrix} \sim \begin{bmatrix} 1 & \omega^2 & \omega \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}.$$

Thus, $x_i, y_i = 1$ for all i. But, for each of the four matrices B_1, B_2, B_3, B_4, there exists a 4×4 strongly balanced submatrix (i.e., each row contains the entries $1, \omega, \omega^2$). To find these submatrices, in each case remove the first row. For B_1 and B_4, remove the first column. For B_2 and B_3, remove the third and second columns, respectively. Thus A is not ray-nonsingular.

3.5 Figures and Tables

Below are graphical representations of $R(0,0) \cap R(\alpha, \beta)$ according to the 24 forms of $[1\, e^{i\alpha}\, e^{ib}]$ in Table 3.1.

Figure 3.3: $R(0,0) \cap R(\alpha, \beta)$ for Forms (1) – (4)

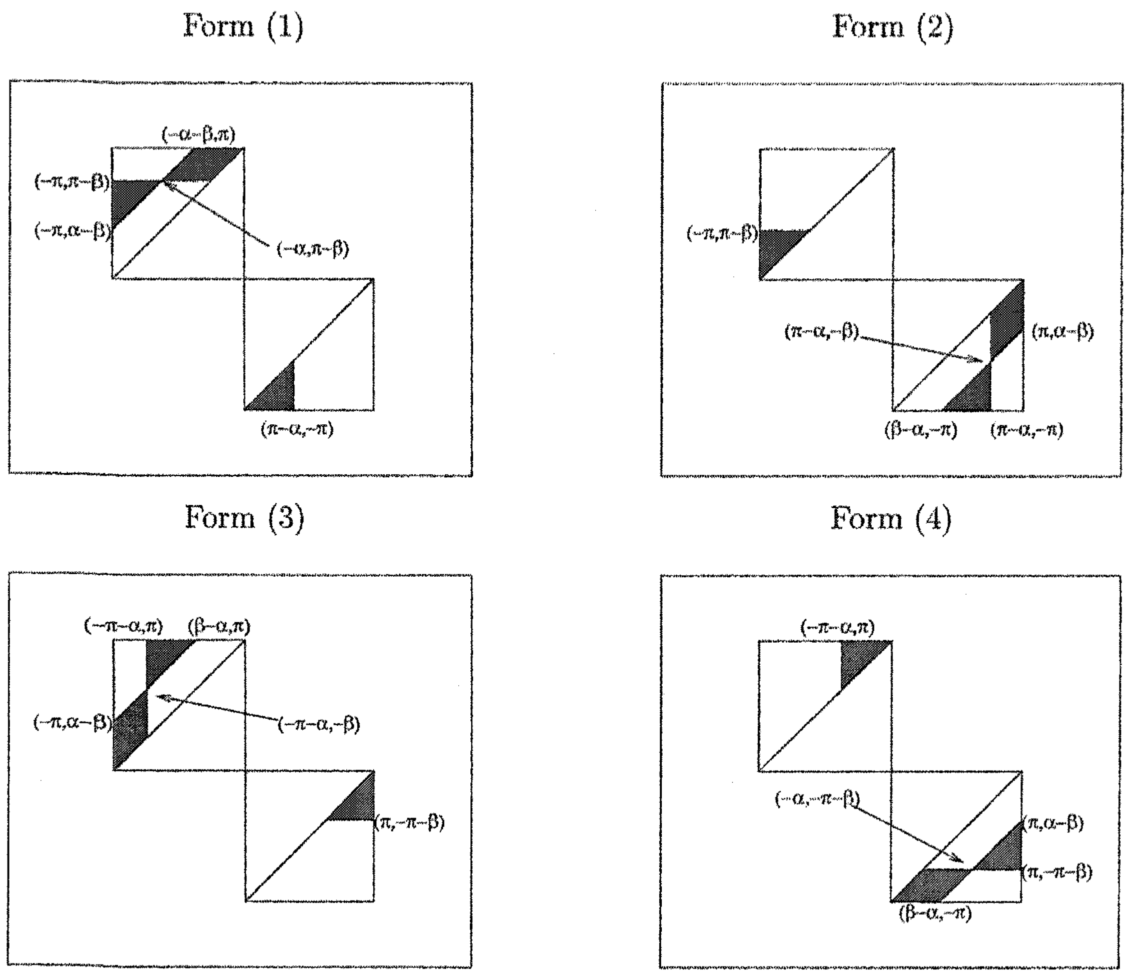
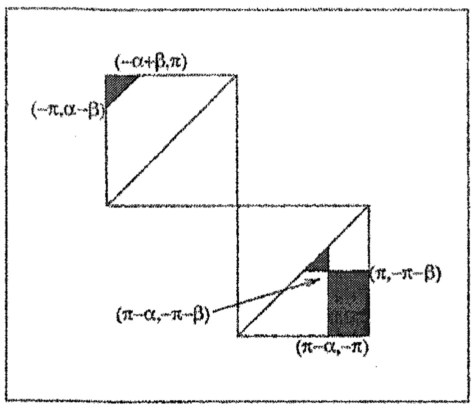
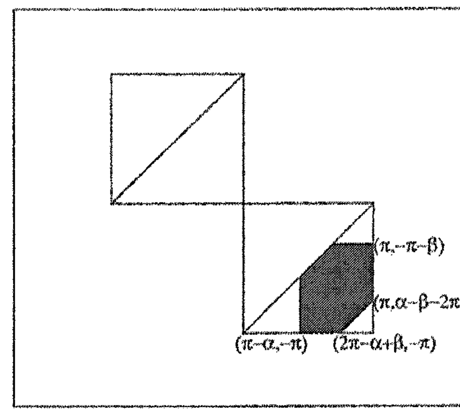


Figure 3.4: $R(0,0) \cap R(\alpha,\beta)$ for Forms (5) – (10)

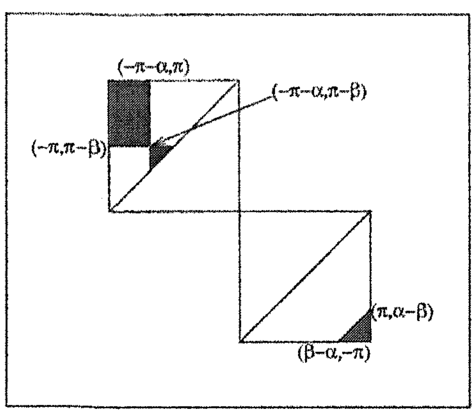
Form (5)



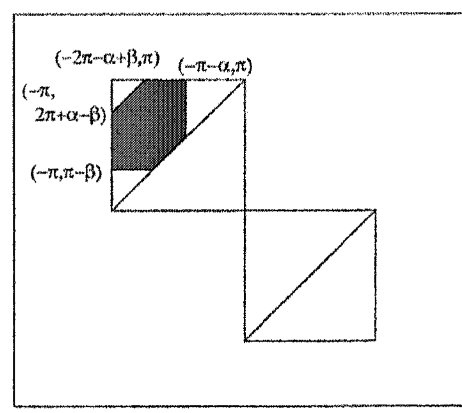
Form (6)



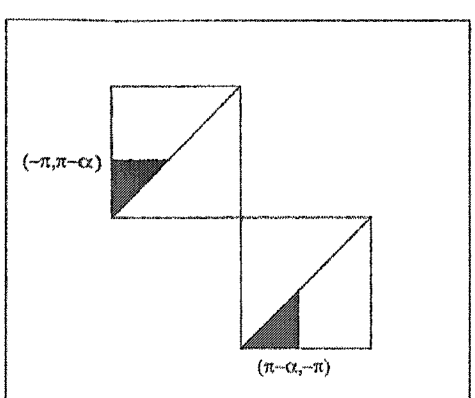
Form (7)



Form (8)



Form (9)



Form (10)

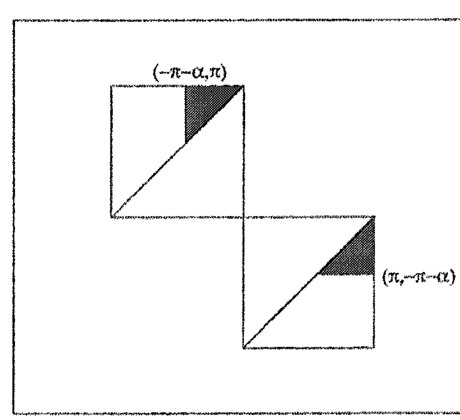


Figure 3.5: $R(0,0) \cap R(\alpha, \beta)$ for Forms (11) - (C4)

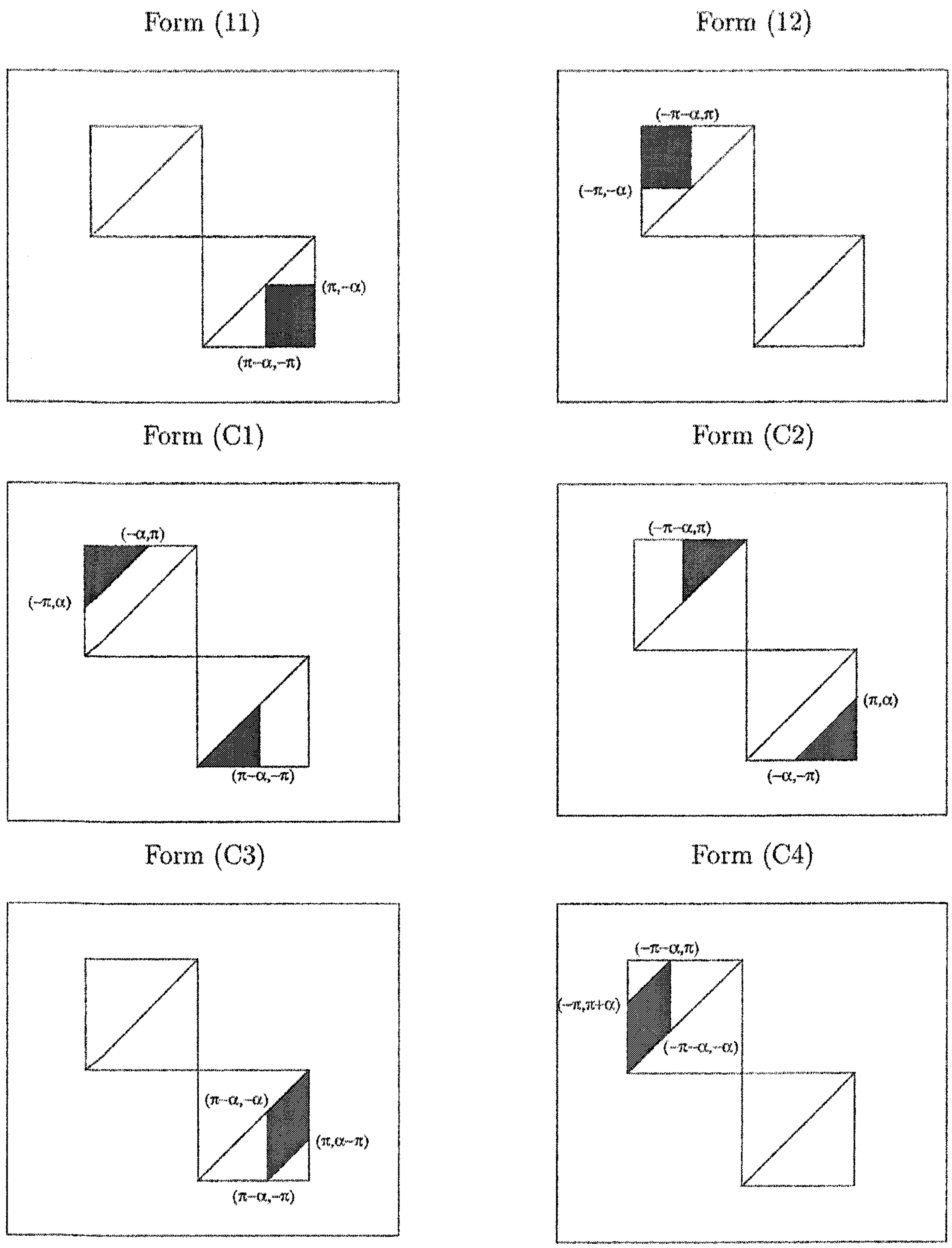


Figure 3.6: $R(0,0) \cap R(\alpha,\beta)$ for Forms (C5) – (C12)

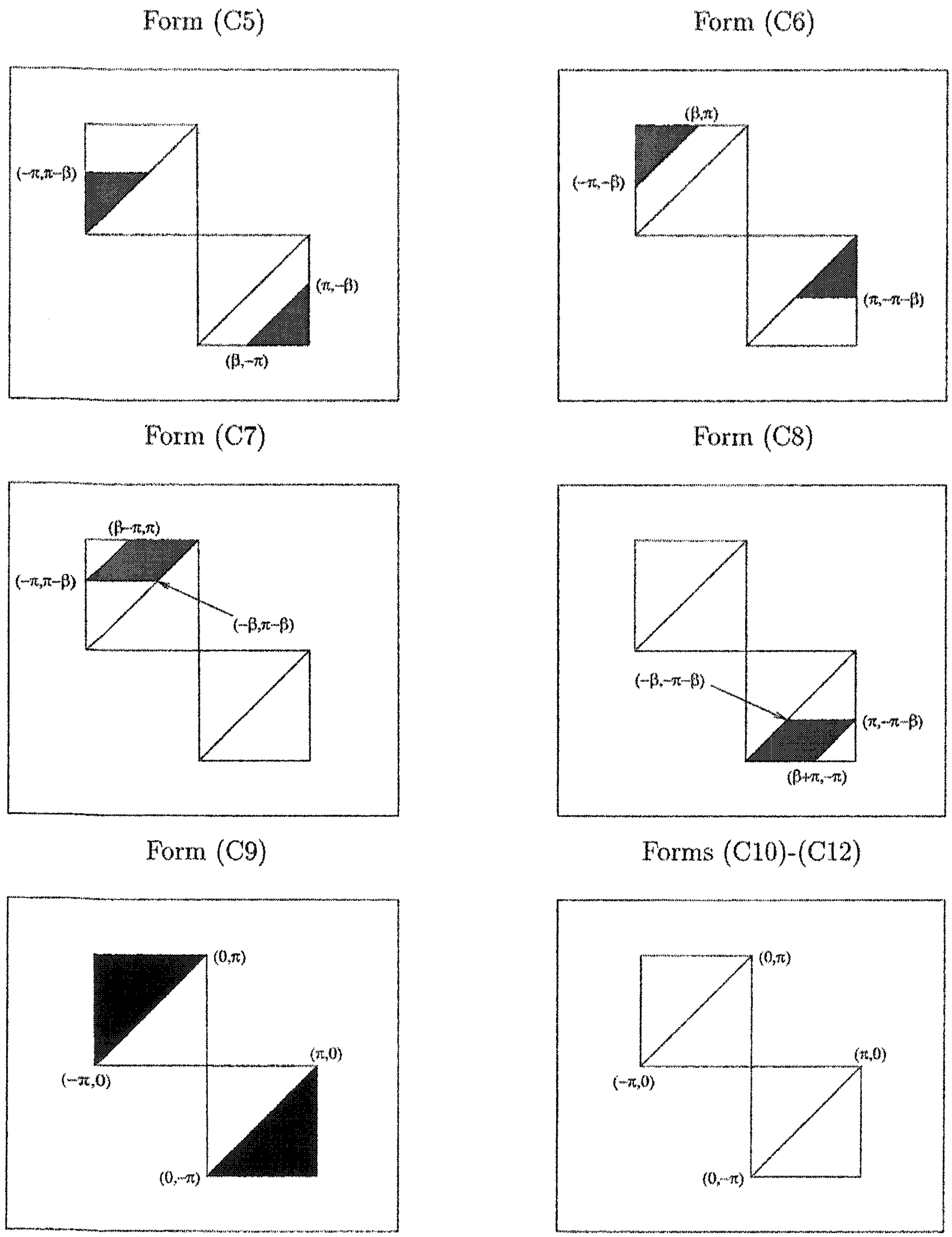


Table 3.2: Intersection of solution sets.

	1	2	3	4	5	6	7	8	9	10	11	12	C1	C2	C3	C4	C5	C6	C7	C8
1	1																			
2	c	1																		
3	c	1	1																	
4	1	c	c	1																
5	c	c	c	c	1															
6	c	1	c	1	1	1														
7	c	c	c	c	1	c	1													
8	1	c	1	c	c	$\emptyset$	1	1												
9	1	1	1	1	c	c	c	c	1											
10	1	1	1	1	c	c	c	c	c	1										
11	c	1	c	1	1	1	1	$\emptyset$	c	c	1									
12	1	c	1	c	1	$\emptyset$	1	1	c	c	$\emptyset$	1								
C1	1	c	c	1	1	c	1	c	1	c	c	1	1							
C2	1	c	c	1	1	c	1	c	c	1	1	c	c	1						
C3	c	1	1	1	1	1	c	$\emptyset$	c	1	1	$\emptyset$	c	c	1					
C4	1	1	1	c	c	$\emptyset$	1	1	1	c	$\emptyset$	1	c	c	$\emptyset$	1				
C5	c	1	1	c	1	c	1	c	1	c	1	c	c	1	c	1	1			
C6	c	1	1	c	1	c	1	c	c	1	c	1	1	c	1	c	c	1		
C7	1	c	1	1	c	$\emptyset$	1	1	c	1	$\emptyset$	1	c	1	$\emptyset$	1	c	c	1	
C8	1	1	c	1	1	1	c	$\emptyset$	1	c	1	$\emptyset$	1	c	1	$\emptyset$	c	c	$\emptyset$	1

Table 3.3: Conditions for empty intersection of the two solution sets.

Form of $[1\ e^{i\alpha_1}\ e^{i\beta_1}]$	Form of $[1\ e^{i\alpha_2}\ e^{i\beta_2}]$	Condition on $\alpha_1, \alpha_2, \beta_1, \beta_2$	Simplification
1	6	$\pi - \alpha_1 \leq \pi - \alpha_2$	$\alpha_2 \leq \alpha_1$
1	11	$\pi - \alpha_1 \leq \pi - \alpha_2$	$\alpha_2 \leq \alpha_1$
6	9	$\pi - \alpha_2 \leq \pi - \alpha_1$	$\alpha_1 \leq \alpha_2$
6	10	$-\pi - \beta_1 \leq -\pi - \beta_2$	$\beta_2 \leq \beta_1$
6	C1	$\pi - \alpha_2 \leq \pi - \alpha_1$	$\alpha_1 \leq \alpha_2$
6	C5	$2\pi - \alpha_1 + \beta_1 \leq \beta_2$	$\beta_1 - \beta_2 + 2\pi \leq \alpha_1$
6	C6	$-\pi - \beta_1 \leq -\pi - \beta_2$	$\beta_2 \leq \beta_1$
9	11	$\pi - \alpha_1 \leq \pi - \alpha_2$	$\alpha_2 \leq \alpha_1$
9	C7	$\pi - \alpha_1 = \pi - \beta_1 \leq \pi - \beta_2$	$\beta_2 \leq \alpha_1 = \beta_1$
10	12	$-\pi - \alpha_2 \leq -\pi - \alpha_1$	$\alpha_1 \leq \alpha_2$
10	C1	$-\alpha_2 \leq -\pi - \alpha_1 = -\pi - \beta_1$	$\beta_1 + \pi = \alpha_1 + \pi \leq \alpha_2$
10	C5	$-\beta_2 \leq -\pi - \alpha_1 = -\pi - \beta_1$	$\beta_1 + \pi = \alpha_1 + \pi \leq \beta_2$
10	C8	$-\pi - \beta_2 \leq -\pi - \alpha_1 = -\pi - \beta_1$	$\beta_1 = \alpha_1 \leq \beta_2$
11	C6	$-\pi - \beta_1 = -\alpha_1 \leq -\pi - \beta_2$	$\beta_2 \leq \beta_1 = \alpha_1 - \pi$
12	C5	$\pi - \beta_2 \leq \pi - \beta_1 = -\alpha_1$	$\alpha_1 + \pi = \beta_1 \leq \beta_2$
C1	C5	$\pi - \beta_2 \leq \alpha_1$	$\pi \leq \alpha_1 + \beta_2$
C3	C5	$-\beta_2 \leq \alpha_1 - \pi$	$\pi \leq \alpha_1 + \beta_2$
C5	C7	$\pi - \beta_1 \leq \pi - \beta_2$	$\beta_2 \leq \beta_1$
C5	C8	$\beta_2 + \pi \leq \beta_1$	$\beta_2 + \pi \leq \beta_1$
C6	C7	$\beta_1 \leq \beta_2 - \pi$	$\beta_1 \leq \beta_2 - \pi$
C6	C8	$\pi - \beta_2 \leq \pi - \beta_1$	$\beta_1 \leq \beta_2$

Chapter 4

Finite Reflection Groups

The following chapter represents work found in [31]. Let V be a Euclidean space and let $\text{End}(V)$ be the algebra of linear endomorphisms on V. An operator $T \in \text{End}(V)$ is a *reflection* if there exists a unit vector $u \in V$ such that $T(v) = v - 2(v,u)u$ for all $v \in V$. A group G of invertible operators in $\text{End}(V)$ is a *reflection group* if it is generated by a set of reflections. The study of reflection groups has motivations and applications in many areas, and the theory is quite well developed; see [4, 8].

4.1 Introduction and Background

Recently, there has been considerable interest in characterizing those linear operators $\phi : \text{End}(V) \to \text{End}(V)$ such that

$$\phi(G) = G. \tag{4.1.1}$$

In other words, ϕ *preserves* G. Wei [48] showed that a linear operator $\phi : \mathrm{End}(V) \to \mathrm{End}(V)$ preserves $G = O(V)$, the group of orthogonal operators on V, if and only if there exist $P, Q \in G$ such that ϕ has the form

$$X \mapsto PXQ \quad \text{or} \quad X \mapsto PX^*Q. \tag{4.1.2}$$

Here, X^* is the adjoint operator of X acting on V so that $(Xu, v) = (u, X^*v)$ for all $u, v \in V$. (Once a basis is chosen, we can replace X^* with X^t.) We are interested in the preservers of the finite reflection groups, which consist of $\mathbf{A}_n$, $\mathbf{B}_n$, $\mathbf{D}_n$, $I_2(n)$, $\mathbf{H}_3$, $\mathbf{H}_4$, $\mathbf{F}_4$, $\mathbf{E}_8$, $\mathbf{E}_7$ and $\mathbf{E}_6$; see [4, p. 76]. Note these are all subgroups of $O(V)$. In [36], it was shown that the same result holds for $G = \mathbf{A}_n$. In [35], the authors reproved this result using a similar approach, and considered the problems for the cases when $G = \mathbf{B}_n, \mathbf{D}_n$ and $\mathbf{I}_2(n)$. For $\mathbf{D}_n$ and $\mathbf{I}_2(n)$, $\phi : \mathrm{End}(V) \to \mathrm{End}(V)$ is a linear operator satisfying (4.1.1) if and only if there exist P and Q in the normalizer $N(G) \leq O(V)$ of G such that ϕ has the form (4.1.2). The same statement is true for $G = O(V)$ and $\mathbf{A}_n$ because $N(G) = G$ in these cases. However, the situation for $G = \mathbf{B}_n$ is different. Suppose $G = \mathbf{B}_n$ is viewed as the group of $n \times n$ signed permutation matrices, i.e., product of diagonal orthogonal matrices and permutation matrices, acting on $V = \mathbf{R}^n$, and $\mathrm{End}(V)$ is identified with the set $M_n(\mathbf{R})$ of $n \times n$ real matrices. Then a linear operator $\phi : M_n(\mathbf{R}) \to M_n(\mathbf{R})$ satisfies (4.1.1) if and only if there exist $P, Q \in G$ and $R = (r_{ij}) \in M_n(\mathbf{R})$ with $r_{ij} \in \{1, -1\}$ such that ϕ has the form

$$X \mapsto R \circ (PXQ) \qquad \text{or} \qquad X \mapsto R \circ (PX^tQ),$$

where $Y \circ Z$ denotes the Schur (entry-wise) product of two matrices $Y, Z \in M_n(\mathbf{R})$.

In this thesis, we consider the problem for the remaining cases, namely, $G = \mathbf{H}_3$, $\mathbf{H}_4$, $\mathbf{F}_4$, $\mathbf{E}_8$, $\mathbf{E}_7$ and $\mathbf{E}_6$, and confirm that a linear operator $\phi : \mathrm{End}(V) \to \mathrm{End}(V)$ satisfies (4.1.1) if and only if there exist $P, Q \in N(G)$ such that (4.1.2) holds.

One may also study the more difficult problem of characterizing linear operators $\phi : \mathrm{End}(V) \to \mathrm{End}(V)$ such that $\phi(G) \subseteq G$. When $G = O(n)$, such a linear map has the usual form (4.1.2) except when $n = 2, 4, 8$, and there are singular maps ϕ satisfying (4.1.1) in these cases; see [48] for details. Furthermore, one may consider other subsets $\mathcal{S}$ of $\mathrm{End}(V)$ related to G and linear maps $\phi : \mathrm{End}(V) \to \mathrm{End}(V)$ such that $\phi(\mathcal{S}) = \mathcal{S}$ and $\phi(\mathcal{S}) \subseteq \mathcal{S}$; see [10, 35, 36]). All of these can be viewed as studies of linear preserver problems related to groups and algebraic sets; see [42, Chapter 4].

This chapter is organized as follows. We present some preliminary results and describe some basic strategies of our proofs in the next section. In Sections 3 – 8, we prove our preserver results for $G = \mathbf{H}_3$, $\mathbf{H}_4$, $\mathbf{F}_4$, $\mathbf{E}_8$, $\mathbf{E}_7$, and $\mathbf{E}_6$, respectively. In each of these sections, we describe a natural matrix realization of G, and possible inner products (X, Y) for elements $X, Y \in G$. These results are then used to solve the corresponding preserver problem. For $G = \mathbf{E}_7$ and $\mathbf{E}_6$, we work on their 8×8 matrix realizations (as subgroups of $\mathbf{E}_8$). Some matlab programs used in our proofs are included in Section 9.

In our discussion, denote by $\{e_1, \ldots, e_n\}$ the standard basis for $\mathbf{R}^n$, $e = \sum_{j=1}^n e_j$, and $E_{ij} = e_i e_j^t \in M_n(\mathbf{R})$. If V is equal to (or identified with) $\mathbf{R}^n$, then $\mathrm{End}(V)$ is equal to (or identified with) $M_n(\mathbf{R})$, which is also a Euclidean space with inner product defined by $(X, Y) = \text{tr}\,(XY^t)$.

It is worth noting that even though the general strategies of our proofs can be easily described, see Section 2, it requires a lot of effort and technical details to prove our results. It would be nice if there are shorter conceptual proofs for our results.

4.2 Preliminary Results

Denote by $O(\text{End}(V))$ the group of orthogonal operators on $\text{End}(V)$ preserving the inner product. We have the following result; see [35, Corollaries 2.2].

Proposition 4.1 *Let G be a finite reflection group acting irreducibly on V. The collection of linear maps $\phi : \text{End}(V) \to \text{End}(V)$ satisfying $\phi(G) = G$ form a subgroup of $O(\text{End}(V))$.*

General Procedures and Strategies

We briefly describe some general procedures and strategies in our proofs in the next few Sections.

GP1. To find a matrix realization of the given reflection group G, we use the standard root systems in $\mathbf{R}^n$ described in [4, p.76] to construct some basic reflections $I_n - 2xx^t$, and their products until we get all the elements in G. Very often, we partition the group G into different subsets to facilitate future discussion.

GP2. Using the matrix realization in GP1, we determine some possible inner products $r = (X, Y)$ for elements $X, Y \in G$. For each r, we define

$$\mathcal{S}_r = \{X \in G : (I, X) = r\}$$

which is used in the proof of the linear preserver result.

GP3. To characterize $\phi : M_n(\mathbf{R}) \to M_n(\mathbf{R})$ such that $\phi(G) = G$, we can always assume that $\phi(I_n) = I_n$. Otherwise, we can replace ϕ by a mapping of the form

$$X \mapsto \phi(I_n)^{-1}\phi(X).$$

By Proposition 4.1, we see that $\phi(\mathcal{S}_r) = \mathcal{S}_r$, where $\mathcal{S}_r$ is defined as in GP2. Then we show that there is an overgroup $\tilde{G}$ of G so that one can strategically modify ϕ by a finite sequence of mappings of the form

$$X \mapsto P^t\phi(X)P \qquad \text{or} \qquad X \mapsto P^t\phi(X)^tP \tag{4.2.3}$$

by $P \in \tilde{G}$ so that the resulting map is the identity map on $M_n(\mathbf{R})$. It will then follow that the original ϕ has the desired form.

GP4. Using our results, one can show that the group $\tilde{G}$ in GP3 is $N(G)$, the normalizer of G in $O(V)$, as follows. By our linear preserver result, if ϕ satisfies $\phi(I_n) = I_n$ and $\phi(G) = G$ then ϕ has the form

$$X \mapsto P^tXP \qquad \text{or} \qquad X \mapsto P^tX^tP,$$

for some P in a certain group $\tilde{G}$. Since the mapping $X \mapsto P^tXP$ sends G onto itself for any $P \in \tilde{G}$, we see that $\tilde{G} \leq N(G)$. Now, if $Q \in N(G)$ then the mapping ϕ

defined by $X \mapsto Q^t X Q$ satisfies $\phi(G) = G$. By our linear preserver result, there exists $P \in \tilde{G}$ such that

$$P^t X P = Q^t X Q \text{ for all } X \in G \qquad \text{or} \qquad P^t X^t P = Q^t X Q \text{ for all } X \in G.$$

If the latter case holds, then $XPQ^tX = PQ^t$ for all $X \in G$, which is impossible; if the former case holds, then one readily shows that $P = Q$. Thus, we get the reverse inclusion $N(G) \leq \tilde{G}$.

GP5. To study $\mathbf{E}_8, \mathbf{E}_7$ and $\mathbf{E}_6$, we first use strategies GP1 - GP4 to handle $\mathbf{E}_8 \subset M_8(\mathbf{R})$. Then we identify $\mathbf{E}_7 \subset M_7(\mathbf{R})$ as a subgroup $\mathcal{E}_7$ of $\mathbf{E}_8 \subset M_8(\mathbf{R})$ by the mapping

$$A \mapsto U^t \begin{pmatrix} 1 & 0 \\ 0 & A \end{pmatrix} U \in \mathbf{E}_8$$

for some suitable orthogonal matrix $U \in M_8(\mathbf{R})$. To characterize a linear map $\psi : M_7(\mathbf{R}) \to M_7(\mathbf{R})$ such that $\psi(\mathbf{E}_7) = \mathbf{E}_7$, we consider an affine map ϕ induced by ψ on the affine space generated by $\mathcal{E}_7$. We use a similar idea to investigate $\mathbf{E}_6$.

4.3 $\mathbf{H}_3$

4.3.1 Matrix realization

The group $\mathbf{H}_3$ has $2^3 \cdot 3 \cdot 5 = 120$ elements; see [4, p.80]. Using the standard root systems (see [4, p.76]) of $\mathbf{H}_3$ in $\mathbf{R}^3$, we see that $\mathbf{H}_3$ admits a matrix realization in $M_3(\mathbf{R})$ consisting of the following matrices:

(I) 24 matrices of the form PD, where $P \in M_3(\mathbf{R})$ is an even permutation (so P is either the identity or a length 3 cycle) and $D \in M_3(\mathbf{R})$ is a diagonal orthogonal matrix.

(II) 12 matrices of the form PHP^t, where P is a matrix of type (I) and

$$H = I_3 - 2(-b, c, a)^t(-b, c, a) = \begin{pmatrix} a & b & c \\ b & c & -a \\ c & -a & -b \end{pmatrix} \tag{4.3.4}$$

with $a = (1 + \sqrt{5})/4$, $b = (-1 + \sqrt{5})/4$, $c = 1/2$. Note that the diagonals of these matrices have the form $(a, c, -b)$, $(-b, a, c)$ or $(c, -b, a)$, and the sum of the diagonal entries is always one.

(III) 84 matrices of the form QD where Q is a type (II) matrix and D is a diagonal orthogonal matrix not equal to I_3. In fact, each of these seven diagonal matrices D generates a class of twelve matrices, and we get seven different classes. Note that the absolute values of the diagonals are (a, c, b), (b, a, c) or (c, b, a).

4.3.2 Inner product

Since $(X, Y) = (I_3, X^tY)$ for any $X, Y \in \mathbf{H}_3$, we focus on the possible values of (I_3, X) with $X \in \mathbf{H}_3$. If $X \in \mathbf{H}_3$ is type (I), then $(I_3, X) \in \{0, \pm 1, \pm 3\}$; $X \in \mathbf{H}_3$ is of type (II), then $(I_3, X) = 1$; if X is type (III), then $(I_3, X) \in \{0, -1, \pm\sqrt{5}/2, \pm(1+\sqrt{5})/2\}$. Thus, if $X \in \mathbf{H}_3$, then

$$(I, X) \in \{0, \pm 1, \pm\sqrt{5}/2, \pm(1 + \sqrt{5})/2, \pm 3\}.$$

By GP2 in Section 2, for each r in the above set, define

$$\mathcal{S}_r = \{X \in \mathbf{H}_3 : (I_3, X) = r\}. \tag{4.3.5}$$

For example, let $r = 1$. If $X \in \mathcal{S}_1$, then X must of one of the following two forms.

(a) The 3 matrices of type (I), namely,

$$D_1 = \text{diag}\,(-1, 1, 1),\ D_2 = \text{diag}\,(1, -1, 1),\ D_3 = \text{diag}\,(1, 1, -1), \tag{4.3.6}$$

(b) The 12 type (II) matrices.

4.3.3 Linear preservers

Theorem 4.2 *A linear operator $\phi : M_3(\mathbf{R}) \to M_3(\mathbf{R})$ satisfies $\phi(\mathbf{H}_3) = \mathbf{H}_3$ if and only if there exist $P, Q \in \mathbf{H}_3$ such that ϕ has the form*

$$X \mapsto PXQ \quad or \quad X \mapsto PX^tQ.$$

Consequently, $N(\mathbf{H}_3) = \mathbf{H}_3$.

Proof. The assertion on $N(\mathbf{H}_3)$ follows from GP4 in Section 2. The ($\Leftarrow$) part of the first assertion is clear. We consider the ($\Rightarrow$) part. Define $\mathcal{S}_r$ as in (4.3.5). By Proposition 4.1, if ϕ preserves $\mathbf{H}_3$, then ϕ preserves the inner product $(X, Y) = \text{tr}\,(XY^t)$. By GP3 in Section 2, we may assume that $\phi(I_3) = I_3$ and $\phi(\mathcal{S}_r) = \mathcal{S}_r$ for each r. In the following, we will show that ϕ has the form $X \mapsto P^tXP$ or $X \mapsto P^tX^tP$ for some $P \in \mathbf{H}_3$. We shall use the matrices D_1, D_2, D_3 and H defined in §3.1 − 3.2.

First, consider $\phi(D_j) = Y_j$ for some $j = 1, 2, 3$. Then $Y_j \in \mathcal{S}_1$. Since $\phi(I_3) = I_3$ and $(D_1 + D_2 + D_3)/2 = I$, we have $(Y_1 + Y_2 + Y_3)/2 = I$. We consider 2 cases depending on whether $\phi(D_1)$ is a type (a) or type (b) matrix defined in §3.2

Case 1. Suppose Y_1 is a type (a) matrix. Then $(Y_1 + Y_2 + Y_3)/2 = I$ implies that all Y_j are type (a) matrices. We can assume that $Y_1 = D_1$; otherwise, replace ϕ by a mapping of the form $X \mapsto Q\phi(X)Q^t$ for a suitable even permutation matrix Q. Then

$$\{\phi(D_2), \phi(D_3)\} = \{D_2, D_3\}.$$

We will show that $\phi(D_i) = D_i$ for $i = 2, 3$.

Suppose that $\phi(X) = Y$ for some $X, Y \in \mathbf{H}_3$. Since ϕ fixes I_3 and D_1, $(X, I_3) = (Y, I_3)$ and $(X, D_1) = (Y, D_1)$. It follows that $\operatorname{tr}(X) = \operatorname{tr}(Y)$ and

$$2(X, E_{11}) = (X, I_3 - D_1) = (Y, I_3 - D_1) = 2(Y, E_{11}).$$

Now, consider

$$\mathcal{T} = \{X \in \mathcal{S}_1 : (I_3, X) = 1,\ (X, E_{11}) = a\} = \{H\} \cup \{D_i H D_i : i = 1, 2, 3\}$$

where H is the matrix in (4.3.4). Then $\phi(\mathcal{T}) = \mathcal{T}$, and thus $\phi(H) \in \mathcal{T}$. We may assume that $\phi(H) = H$, otherwise replace ϕ with $X \mapsto D_i\phi(X)D_i$. Since

$$(H, \phi(D_2)) = (\phi(H), \phi(D_2)) = (H, D_2) \neq (H, D_3),$$

it follows that $\phi(D_2) = D_2$, and thus $\phi(D_3) = D_3$. So, we have shown that the modified mapping ϕ fixes X for $X = I_3, D_1, D_2, D_3, H$.

Since $\phi(D_i) = D_i$ and ϕ preserves inner product, we see that $(D_i, X) = (D_i, \phi(X))$ for all $i = 1, 2, 3$. Thus $\phi(X)$ and X have the same diagonal. Consider the four matrices with diagonal $(-a, c, -b)$, namely,

$$X_1 = D_1H, \quad X_2 = HD_1 = X_1^t, \quad X_3 = -D_2HD_3, \quad X_4 = -D_3HD_2 = X_3^t.$$

Then $\phi(X_1) = X_j$ for some $j \in \{1, 2, 3, 4\}$. Since

$$(\phi(X_1), H) = (\phi(X_1), \phi(H)) = (X_1, H) = (X_2, H) \neq (X_3, H) = (X_4, H),$$

we see that $\phi(X_1) \in \{X_1, X_2\}$. We may assume that $\phi(X_1) = X_1$; otherwise, replace ϕ with the mapping $X \mapsto \phi(X)^t$. Then $\phi(X_2) = X_2$. Furthermore, we have $\phi(X_3) \in \{X_3, X_4\}$. Since

$$(X_1, \phi(X_3)) = (\phi(X_1), \phi(X_3)) = (X_1, X_3) \neq (X_1, X_4),$$

we see that $\phi(X_3) = X_3$. As a result, we have $\phi(X_i) = X_i$ for $i = 1, 2, 3, 4$.

Next, consider the four matrices with diagonal $(a, -c, -b)$, namely,

$$X_5 = D_2H, \quad X_6 = HD_2, \quad X_7 = -D_1HD_3, \quad X_8 = -D_3HD_1.$$

Since $(H - X_1, X_i) \neq (H - X_1, X_j)$ for $5 \leq i < j \leq 8$, we have $\phi(X_i) = X_i$ for $i = 5, 6, 7, 8$.

Now, we have $\phi(X) = X$ for $X \in \{D_1, D_2, D_3, H, X_1, \ldots, X_8\}$, which is a spanning set of $M_3(\mathbf{R})$; for example, it can be checked using MATLAB as shown in the last section. Thus $\phi(X) = X$ for all $X \in M_3(\mathbf{R})$.

Case 2. If Y_1 is a type (b) matrix, then we may replace ϕ by a mapping of the form $X \mapsto P\phi(X)P^t$ for a type (I) matrix P and assume that $Y_1 = H$. Then replace ϕ by the mapping $X \mapsto HQ^tD_1\phi(X)D_1QH$ with $Q = E_{12} + E_{23} + E_{31}$; we see that $\phi(D_1) = D_1$, and we are back to case 1. □

4.4 $\mathbf{H}_4$

4.4.1 Matrix realization

Note that $\mathbf{H}_4$ has $2^6 \cdot 3^2 \cdot 5^2$ elements; see [4, p.80]. Let

$$a = (1+\sqrt{5})/4, \quad b = (-1+\sqrt{5})/4, \quad c = 1/2.$$

Using GP1 in Section 2 and the standard root systems of $\mathbf{H}_4$ in $\mathbf{R}^4$ (see [4, p.76]), we see that $\mathbf{H}_4$ contains the following two matrices:

$$A = I - ee^t/2 = \frac{1}{2}\begin{pmatrix} 1 & -1 & -1 & -1 \\ -1 & 1 & -1 & -1 \\ -1 & -1 & 1 & -1 \\ -1 & -1 & -1 & 1 \end{pmatrix}, \tag{4.4.7}$$

and

$$B = I_4 - 2(0,-b,c,a)^t(0,-b,c,a) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & a & b & c \\ 0 & b & c & -a \\ 0 & c & -a & -b \end{pmatrix}. \tag{4.4.8}$$

Using these two matrices, we can describe the matrices in $M_4(\mathbf{R})$ as follows.

(I) $4!2^3 = 2^6 3$ matrices of the form PD, where P is an even permutation, and D is a diagonal orthogonal matrix. Note that $(I_4, P) \in \{0, \pm 1, \pm 4\}$.

(II) $2^7 3$ matrices of the form PAQ, where A is the matrix in (4.4.7), and P, Q are matrices of type (I). Note that

$$(I_4, PAQ) \in \{0, \pm 1, \pm 2\}.$$

(III) $2^{10}3$ matrices of the form PBQ, where B is the matrix in (4.4.8), and P, Q are matrices of type (I). The counting is done as follows. For a matrix of the form PBQ, each P and Q has $2^4 12$ choices. However, $PBQ = RBS$ if and only if $R^t PBQS^t = B$. So, we have to count pairs of (X, Y) such that $XBY = B$. One can check that $XBY = B$ if and only if $X = [r] \oplus U$ and $Y = [r] \oplus V$, where $r = \pm 1$ and (U, V) is one of the following pairs:

$$\pm(I_3, I_3),\ \pm(-E_{13} + E_{21} + E_{32}, E_{13} + E_{21} - E_{32}),$$

$$\pm(E_{12} + E_{23} - E_{31}, E_{12} + E_{23} - E_{31}).$$

So, there are 12 pairs of matrices (X, Y), and the total number of type (III) matrices is $(2^4 12)^2/12 = 2^{10}3$. Note that

$$(I_4, PBQ) \in \{0, \pm 1, \pm 2, (\pm 1 \pm \sqrt{5})/2, (\pm 3 \pm \sqrt{5})/2\}.$$

(IV) $2^{11}3$ matrices of the form PCQ, where P, Q are matrices of type (I), and

$$C = B \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} B = \begin{pmatrix} 0 & a & b & c \\ a & b & 0 & -c \\ b & 0 & -a & c \\ c & -c & c & c \end{pmatrix}.$$

The counting is done as follows. For a matrix of the form PCQ, each P and Q has $2^4 12$ choices. However, $PCQ = RCS$ if and only if $R^t PCQS^t = C$. So, we have to count pairs of (X, Y) such that $XCY = C$. One can check that $XCY = C$ if and only if $X = Y = \pm(U \oplus [1])$ with $U = I_3$, $E_{13} - E_{21} - E_{32}$, or $-E_{12} - E_{23} + E_{31}$. So, there are 6 pairs of such matrices (X, Y), and the total number of class (IV) matrices is $(2^4 12)^2/6 = 2^{11}3$. Note that

$$(I_4, PCQ) \in \{0, \pm 1, (\pm 1 \pm \sqrt{5})/2, (\pm 3 \pm \sqrt{5})/2\}.$$

(V) $3 \cdot 2^6 \cdot 24$ matrices of the form PEQ, where P and Q are type (III) matrices and

$$\begin{aligned} E &= (E_{12} + E_{21} + E_{34} - E_{43})B(E_{14} + E_{23} - E_{32} + E_{41})B \\ &= \begin{pmatrix} c & 0 & b & -a \\ 0 & c & -a & -b \\ -b & a & c & 0 \\ a & b & 0 & c \end{pmatrix}. \end{aligned} \tag{4.4.9}$$

The counting is done as follows. For a matrix of the form PEQ, each P and Q has $2^4 12$ choices. However, $PEQ = RES$ if and only if $R^t PEQS^t = E$. So, we have to count pairs of (X, Y) such that $XEY = E$. One can check that $XEY = E$ if and only if $X = Y^t$ is the plus or minus of one of the following:

$$I_4, E_{12} - E_{21} + E_{34} - E_{43}, E_{13} + E_{24} - E_{31} - E_{42}, E_{14} - E_{23} + E_{32} - E_{41}.$$

So, there are 8 pairs of such matrices (X, Y), and the total number of class (V) matrices is $(2^4 12)^2/8 = 3 \cdot 2^6 \cdot 24$. One checks that

$$(I_4, PEQ) \in \{0, \pm 1, \pm 2, (\pm 1 \pm \sqrt{5})/2, \pm 1 \pm \sqrt{5}\}.$$

4.4.2 Inner product

By the discussion in the last subsection, if $X \in \mathbf{H}_4$, then

$$(I_4, X) \in \{0, \pm 1, \pm 2, (\pm 1 \pm \sqrt{5})/2, (\pm 3 \pm \sqrt{5})/2, \pm 1 \pm \sqrt{5}, \pm 4\}.$$

By GP2 in Section 2, for each r in the above set, define

$$\mathcal{S}_r = \{Y \in \mathbf{H}_4 : (I_4, Y) = r\}. \tag{4.4.10}$$

Then $\mathcal{S}_2$ consists of matrices of the following forms.

(a) The 4 diagonal matrices, namely

$$D_i = I_4 - 2E_{ii}, \qquad i = 1, 2, 3, 4. \tag{4.4.11}$$

(b) The 24 matrices of the form DA_iD for $i = 1, 2, 3$ where $D = \text{diag}\,(1, \pm 1, \pm 1, \pm 1)$, $A_1 = A$ defined in (4.4.7),

$$A_2 = \frac{1}{2}\begin{pmatrix} 1 & -1 & -1 & -1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \\ 1 & -1 & 1 & 1 \end{pmatrix} \qquad \text{and} \qquad A_3 = A_2^t.$$

(c) The 48 type (III) matrices with diagonal entries $1, a, -b, c$ in a certain order. Note that these must be of the form PBP^t where P is of type (I). To see this, note that if P and Q are type (I) matrices such that PBQ has diagonal entries $1, a, -b, c$, then removing the row and column containing the entry 1, we get a type (II) matrix of Section 3.1. Hence, we see that $Q = P^t$.

(d) The 24 type (V) matrices of the form PEP^t where P is a type (I) matrix. This conjugation will leave the diagonal entries (namely c, c, c, c) on the diagonal.

4.4.3 Linear preservers

Theorem 4.3 *A linear operator $\phi : M_4(\mathbf{R}) \to M_4(\mathbf{R})$ satisfies $\phi(\mathbf{H}_4) = \mathbf{H}_4$ if and only if there exist $P, Q \in \mathbf{H}_4$ such that ϕ has the form*

$$X \mapsto PXQ \quad \text{or} \quad X \mapsto PX^tQ.$$

Consequently, $N(\mathbf{H}_4) = \mathbf{H}_4$.

Proof. The assertion on $N(\mathbf{H}_4)$ follows from GP4 in Section 2. The ($\Leftarrow$) part of the first assertion is clear. We consider the ($\Rightarrow$) part. Define $\mathcal{S}_r$ as in (4.4.10). By Proposition 4.1, if ϕ preserves $\mathbf{H}_4$, then ϕ preserves the inner product $(X, Y) = \operatorname{tr}(XY^t)$. By GP3 in Section 2, we may assume that $\phi(I_4) = I_4$ and $\phi(\mathcal{S}_r) = \mathcal{S}_r$ for each r. In the following, we will show that ϕ has the form $X \mapsto P^tXP$ or $X \mapsto P^tX^tP$ for some $P \in \mathbf{H}_4$. We shall frequently use the matrices D_1, D_2, D_3, D_4, A_1, A_2, A_3, B and E as defined in §4.1 – 4.2 as well as the classification of elements of $\mathcal{S}_2$ as types (a), (b), (c) and (d) as defined in §4.2. Furthermore, denote by $D_{ij} = D_iD_j$.

For E defined as in (4.4.9), since $D_{12}ED_{12} = E^t$ and $E + E^t = I_4$, the elements of (d) can be paired up such that $X + X^t = I_4$, where both X and X^t are in (d). Also, the same applies for those matrices in (b) of the form DA_iD, where $i = 2, 3$. (For example, $A_2 + A_3 = I_4$). Now consider $\phi(D_i) = Y_i$. Note that since there exists no $X \in \mathcal{S}_2$ such that $D_i + X = I$; thus, Y_i must be of type (a), (c), or type (b) of the form DA_1D. We consider three cases according to these.

Case 1. Suppose that $Y_1 = D_j$. Then replace ϕ with a mapping of the form

$X \mapsto P\phi(X)P^t$ where P is an even permutation such that $\phi(D_1) = D_1$. Note that

$$2(\phi(X), E_{11}) = (\phi(X), I_4 - D_1) = (X, I_4 - D_1) = 2(X, E_{11}).$$

Let $D_1 + X_2 + X_3 + X_4 = 2I_4$ where $X_i \in \mathcal{S}_2$. Since $(X_2 + X_3 + X_4, E_{11}) = 3$, and since 1 is the largest possible value for (X_i, E_{11}), it follows that each X_i is either of type (a) or one of the 12 type (c) with the $(1,1)$ entry equal to one. Thus, either $\phi(D_2) = D_j$ or $\phi(D_2) = Z_2$ where Z_2 is one of the 12 type (c) matrices. If the first case happens, we may assume that $\phi(D_2) = D_2$; otherwise, replace ϕ by a mapping of the form $X \mapsto P\phi(X)P^t$ for a suitable even permutation matrix P such that $(P, E_{11}) = 1$. If the second case happens, then there exists a signed even permutation matrix Q with $(Q, E_{11}) = 1$ such that $Q^t\phi(D_1)Q = B$. Now, replace ϕ by a mapping of the form $X \mapsto BPD_2Q^t\phi(X)QD_2P^tB$ with $P = E_{11} + E_{24} + E_{32} + E_{43}$. Then the resulting map fixes I_4, D_1, D_2.

Recall that $\phi(D_i) = Y_i$ for $i = 1, \ldots, 4$, and $Y_1 + Y_2 + Y_3 + Y_4 = 3I_4$. Thus,

$$\{\phi(D_3), \phi(D_4)\} = \{D_3, D_4\}.$$

Moreover, for $i \in \{1, 2\}$, $(X, E_{ii}) = (\phi(X), \phi(E_{ii})) = (\phi(X), E_{ii})$. Consider the set

$$\mathcal{T} = \{X \in \mathcal{S}_2 : (X, E_{11}) = 1,\ (X, E_{22}) = a\} = \{D_iBD_i : i = 1, 2, 3, 4\}.$$

(Note that $B = D_1BD_1$). Then $\phi(\mathcal{T}) = \mathcal{T}$. If $\phi(B) = D_iBD_i$, then replace ϕ with $X \mapsto D_i\phi(X)D_i$. So, we may assume ϕ fixes B. Now, since $(D_3, B) \neq (D_4, B)$, we have $\phi(D_3) = D_3$ and $\phi(D_4) = D_4$. It then follow that

$$(X, E_{ii}) = (\phi(X), E_{ii}), \qquad i = 1, ..., 4.$$

Since $(B, D_iBD_i) \neq (B, D_jBD_j)$ for $i \neq j$, we have

$$\phi(D_iBD_i) = D_iBD_i, \qquad i = 2, 3, 4.$$

Let $P = E_{12} + E_{23} + E_{31} + E_{44}$, and consider the matrices

$$B_1 = B, \quad B_2 = PBP^t, \quad B_3 = P^tBP.$$

Consider those matrices in $\mathcal{S}_2$ with diagonal $(a, c, 1, -b)$, namely, $D_iB_2D_i$ for $i = 1, 2, 3, 4$ (note that $B_2 = D_3B_2D_3$). Then

$$(B, B_2) = (B, D_1B_2D_1) \neq (B, D_2B_2D_2) = (B, D_4B_2D_4).$$

We may assume that $\phi(B_2) = B_2$. Otherwise, $\phi(B_2) = D_1B_2D_1$ and replace ϕ with $X \mapsto D_1\phi(X)D_1$. Now $\phi(D_2B_2D_2) = D_iB_2D_i$ for either $i = 2$ or $i = 4$. Since $(B_2, D_2B_2D_2) \neq (B_2, D_4B_2D_4)$, we have

$$\phi(D_iB_2D_i) = D_iB_2D_i, \qquad i = 1, 2, 3, 4.$$

The matrices with diagonal $(c, 1, a, -b)$ are $D_iB_3D_i$ for $i = 1, 2, 3, 4$ (note that $B_3 = D_2B_3D_2$). We have

$$(B, B_3) = (B, D_1B_3D_1) \neq (B, D_3B_3D_3) = (B, D_4B_3D_4).$$

But $(B_2, B_3) = (B_2, D_3B_3D_3) \neq (B_2, D_1B_3D_1) = (B_2, D_4B_3D_4)$. Therefore,

$$\phi(D_iB_3D_i) = D_iB_3D_i, \qquad i = 1, 2, 3, 4.$$

Next, consider

$$B_4 = D_3B, \quad B_5 = D_2B_2, \quad \text{and} \quad B_6 = D_1B_3.$$

Their diagonals are $(1, a, -c, -b)$, $(a, -c, 1, -b)$ and $(-c, 1, a, -b)$ respectively. Note that for each $i = 4, 5, 6$, that $D_j B_i D_j$ share diagonal entries, where $j = 1, 2, 3, 4$. Since the triples $((B, D_j B_i D_j)\ (B_2, D_j B_i D_j)\ (B_3, D_j B_i D_j))$ are different for different i, j, one can see that each of these 12 matrices must be mapped to themselves. Thus $\phi(X) = X$ where $X = D_j B_i D_j$ for $j = 1, 2, 3, 4$ and $i = 1, ..., 6$. One readily checks that these 24 matrices span $M_4(\mathbf{R})$; see the last section. So ϕ fixes every matrix in $M_4(\mathbf{R})$.

Case 2. Suppose that Y_1 has the form PBP^t. Then replace ϕ by the mapping of the form $X \mapsto P\phi(X)P^t$. Thus $Y_1 = B$. Then replace ϕ by the mapping $X \mapsto BP^t\phi(X)PB$ where $P = E_{11} + E_{23} + E_{34} + E_{42}$. Thus $\phi(D_1) = D_1$, and we are back to case 1.

Case 3. Suppose that Y_1 has the form DA_1D. Then replace ϕ by the mapping of the form $X \mapsto D\phi(X)D$ where D is such that $\phi(D_1) = A_1$. Then replace ϕ with the mapping of the form $X \mapsto A_1D_1\phi(X)D_1A_1$. Thus $\phi(D_1) = D_1$, and we are back to case 1. □

4.5 $\mathbf{F}_4$

4.5.1 Matrix realization

The group $\mathbf{F}_4$ has $4!2^4 3$ elements (see [4, p.80]) and is generated by $\mathbf{B}_4$ and the matrix

$$A = I - ee^t/2 = \frac{1}{2}\begin{pmatrix} 1 & -1 & -1 & -1 \\ -1 & 1 & -1 & -1 \\ -1 & -1 & 1 & -1 \\ -1 & -1 & -1 & 1 \end{pmatrix}. \tag{4.5.12}$$

Let $\tilde{G}$ be the group in $O(4)$ generated by $\mathbf{B}_4$ and the matrix

$$B = \frac{1}{\sqrt{2}}\left\{\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \oplus \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\right\}. \tag{4.5.13}$$

Then $\tilde{G}$ has $4!2^5 3$ elements. Our result will show that $\tilde{G} = N(\mathbf{F}_4)$ as discussed in GP4 in Section 2.

4.5.2 Inner product

By the discussion in the last subsection, if $X \in \mathbf{F}_4$, then

$$(I_4, X) \in \{0, \pm 1, \pm 2, \pm 4\}.$$

By GP2 in Section 2, for each r in the above set, define

$$S_r = \{Y \in \mathbf{F}_4 : (I_4, Y) = r\}. \tag{4.5.14}$$

The set S_2 consists of matrices of the following forms.

(I) There are 4 diagonal matrices, namely, $D_i = I_4 - 2E_{ii}$, $i = 1, \ldots, 4$.

(II) There are 24 matrices of the form $DP_{ij} \in \mathbf{B}_4$, where P_{ij} is the matrix obtained from I_4 by interchanging the ith and jth rows for $1 \le i < j \le 4$, and D is a diagonal orthogonal matrix such that $\operatorname{tr}(DP_{ij}) = 2$. For example,

$$P_{34} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

(III) There are 48 matrices of the form $DA_1D, \ldots, DA_6D$, where

$$A_1 = \frac{1}{2}\begin{pmatrix} 1 & -1 & -1 & -1 \\ -1 & 1 & -1 & -1 \\ -1 & -1 & 1 & -1 \\ -1 & -1 & -1 & 1 \end{pmatrix}, \quad A_2 = \frac{1}{2}\begin{pmatrix} 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix},$$

$$A_3 = \frac{1}{2}\begin{pmatrix} 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & 1 & 1 \end{pmatrix}, \quad A_4 = \frac{1}{2}\begin{pmatrix} 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 \end{pmatrix},$$

$$A_5 = \frac{1}{2}\begin{pmatrix} 1 & -1 & -1 & -1 \\ 1 & 1 & 1 & -1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 \end{pmatrix}, \quad A_6 = \frac{1}{2}\begin{pmatrix} 1 & -1 & -1 & -1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \\ 1 & -1 & 1 & 1 \end{pmatrix},$$

and

$$D \in \{\operatorname{diag}(1, \delta_1, \delta_2, \delta_3) : \delta_1, \delta_2, \delta_3 \in \{1, -1\}\}.$$

4.5.3 Linear preservers

Theorem 4.4 *A linear operator $\phi : M_4(\mathbf{R}) \to M_4(\mathbf{R})$ on $M_4(\mathbf{R})$ satisfies $\phi(\mathbf{F}_4) = \mathbf{F}_4$ if and only if there exist P, Q in the group $\tilde{G}$ generated by $\mathbf{F}_4$ and B defined in* (4.5.13) *with $PQ \in \mathbf{F}_4$ such that ϕ has the form*

$$X \mapsto PXQ \quad or \quad X \mapsto PX^tQ.$$

Consequently, $N(\mathbf{F}_4) = \tilde{G}$.

Proof. The assertion on $N(\mathbf{F}_4)$ follows from the GP4 in Section 2. The ($\Leftarrow$) part of the first assertion is clear. We consider the ($\Rightarrow$) part. Define $\mathcal{S}_r$ as in (4.5.14). By Proposition 4.1, if ϕ preserves $\mathbf{H}_4$, then ϕ preserves the inner product $(X, Y) = \mathrm{tr}\,(XY^t)$. By GP3 in Section 2, we may assume that $\phi(I_4) = I_4$ and $\phi(\mathcal{S}_r) = \mathcal{S}_r$ for each r. In the following, we will show that ϕ has the form $X \mapsto P^tXP$ or $X \mapsto P^tX^tP$ for some $P \in \tilde{G}$. Throughout this proof we will use the matrices $D_1, D_2, D_3, D_4, A_1, ..., A_6$ and P_{ij} as defined in §5.1 – 5.2. We also refer to matrices in $\mathcal{S}_2$ as types (I), (II) and (III) as defined in §5.2.

Note that the four type (I) matrices $D_1, \ldots, D_4$ are mutually orthogonal matrices satisfying $(D_1 + \cdots + D_4)/2 = I_4$. Let $\phi(D_j) = Y_j$ for $j = 1, \ldots, 4$.

Case 1. If Y_1 is one of the four type (I) matrices, then $(Y_1 + Y_2 + Y_3 + Y_4)/2 = I$ implies that all Y_j are type (I) matrices. We can assume that $Y_j = D_j$ for all $j = 1, \ldots, 4$; otherwise, replace ϕ by a mapping of the form $X \mapsto Q\phi(X)Q^t$ for a suitable permutation matrix Q.

Now note that $(D_j, X) = 1$ for all X in type (III) of $\mathcal{S}_2$ and $j = 1, \ldots, 4$. For $1 \leq i < j \leq 4$, let $\mathcal{P}_{ij}$ be the set of 4 type (II) matrices of the form DP_{ij}. Then for all $X \in \mathcal{P}_{ij}$, $(D_k, X) = 2$ if $k = i, j$ and $(D_k, X) = 0$ otherwise. The same must be true of $\phi(X)$. Thus, $\phi(\mathcal{P}_{ij}) = \mathcal{P}_{ij}$.

Let

$$C_1 = I_2 \oplus \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \in \mathcal{P}_{34} \quad \text{and} \quad \phi(C_1) = I_2 \oplus \begin{pmatrix} 0 & y_1 \\ y_2 & 0 \end{pmatrix} \in \mathcal{P}_{34}.$$

We claim that $y_1 = y_2$. Note that $Z \in \mathcal{S}_2$ satisfies $(C_1, Z) = 1$ if and only if one of the following holds:

(a) Z is one of the type (II) matrices with only one diagonal entry overlapping with those of C_1. There are 16 such matrices having the form DP_{13}, DP_{14}, DP_{23} and DP_{24}, with four choices of diagonal orthogonal matrices D for each P_{ij}.

(b) Z is one of the type (III) matrices such that the $(3,4)$ and $(4,3)$ entries have different signs. There are 32 such matrices having the form DA_jD for $j = 3, 4, 5, 6$, with eight choices of diagonal orthogonal matrices D for each A_j.

As a result, there should be 48 matrices Z in $\mathcal{S}_2$ such that $(\phi(C_1), Z) = 1$. However, if the $(3,4)$ and $(4,3)$ entries of $\phi(C_1)$ have different signs, then $Z \in \mathcal{S}_2$ satisfies $(\phi(C_1), Z) = 1$ can only happen if Z satisfies (a) or

(c) Z is one of the type (III) matrices such that the $(3,4)$ and $(4,3)$ entries have the same sign. there are 16 such matrices having the form DA_jD for $j = 1, 2$, with eight choices of diagonal orthogonal matrices D for each A_j.

Thus, there are only 32 such matrices, which is a contradiction. Therefore, ϕ maps symmetric matrices in $\mathcal{P}_{34}$ to symmetric matrices in $\mathcal{P}_{34}$. Note that one can generalize this argument for all $\mathcal{P}_{ij}$ for all i, j.

We may assume that $\phi(C_1) = C_1$; otherwise, replace ϕ by a mapping of the form $X \mapsto D_4\phi(X)D_4$. Now,

$$C_2 = I_2 \oplus \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \in \mathcal{P}_{34}$$

is not a symmetric matrix in $\mathcal{P}_{34}$, and thus $\phi(C_2) \in \mathcal{P}_{34}$ is not symmetric. We may assume that $\phi(C_2) = C_2$; otherwise, replace ϕ by the mapping $X \mapsto \phi(X)^t$.

Divide type (III) matrices into two subclasses:

$\mathcal{T}_1$ is the set of type (III) matrices of the form PA_iP^t, where $i = 1, 2$ (i.e., $(X, E_{34}) = (X, E_{43})$), and

$\mathcal{T}_2$ is the set of type (III) matrices of the form PA_iP^t, where $i = 3, 4, 5, 6$ (i.e., $(X, E_{34}) = -(X, E_{43})$).

Then $(C_1, X) = 1$ for a type (III) matrix X if and only if $X \in \mathcal{T}_2$. Let

$$C_3 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \oplus I_2, \quad C_4 = [1] \oplus \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \oplus [1].$$

Since the symmetric matrices in $\mathcal{P}_{12}$ are mapped to themselves, we may assume that $\phi(C_3) = C_3$; otherwise, replace ϕ by a mapping of the form $X \mapsto D_1\phi(X)D_1$. Since symmetric elements of $\mathcal{P}_{23}$ are mapped to themselves, we may assume that $\phi(C_4) = C_4$; otherwise, replace ϕ by a mapping of the form $X \mapsto D_{12}\phi(X)D_{12}$.

Next, we show that ϕ fixes $E = E_{12} + E_{23} + E_{34} + E_{41}$. Since $(E, D_j) = 0$ for all $j \in \{1, \ldots, 4\}$, and $(E, X) = 0$ for all $X \in \mathcal{P}_{ij}$ with $(i, j) \in \{(1, 3), (2, 4)\}$, it follows that $\phi(E)$ has a zero in all eight of the nonzero entry found among these eight matrices. Since $(E, C_i) = (-1)^{i-1}$ for $i = 1, 2$, we have $(\phi(E), E_{34}) = 1$ and $(\phi(E), E_{43}) = 0$. So $\phi(E) = \pm E_{12} \pm E_{23} + E_{34} \pm E_{41}$. Since $(E, C_i) = 1$ for $i = 3, 4$, $\phi(E) = E_{12} + E_{23} + E_{34} + E_{41} = E$ or $\phi(E) = E_{12} + E_{23} + E_{34} - E_{41} = \hat{E}$. But $(E, X) = 2$ for exactly one matrix, namely $D_2 A_4 D_2$ in $\mathcal{T}_2$, whereas $(\hat{E}, X) = 2$ for 3 different matrices $D_{24} A_3 D_{24}, D_1 A_5 D_1$, and $D_{24} A_6 D_{24}$ in $\mathcal{T}_2$. Thus, $\phi(E) = E$. A similar argument shows that $\phi(E^t) = E^t$.

Let

$$C_5 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \oplus I_2 \quad \text{and} \quad C_6 = [1] \oplus \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \oplus [1].$$

Since $(E, C_i) = -1$ and $(E, C_i^t) = 1$ for $i \in \{5, 6\}$, it follows that $\phi(C_i) = C_i$ and $\phi(C_i^t) = C_i^t$ for $i \in \{5, 6\}$.

For each $X \in \mathcal{T}_1$ define

$$f(X) = [(I, X), (E, X), (E^t, X), (D_1, X), \ldots, (D_4, X), (C_1, X), \ldots, (C_6, X)].$$

Then one can show (say, using MATLAB) that $f(X) \neq f(Y)$ whenever $X \neq Y$ in $\mathcal{T}_1$. Since ϕ fixes the matrices $I_4, E, E^t, D_1, \ldots, D_4, C_1, \ldots, C_6$, it follows that $\phi(X) = X$ for all $X \in \mathcal{T}_1$. One can check that

$$\mathcal{T}_1 \cup \{D_1, \ldots, D_4, C_1, \ldots, C_6\}$$

span $M_n(\mathbf{R})$; see the last section. Thus, $\phi(X) = X$ for all $X \in M_n(\mathbf{R})$.

Case 2. Suppose Y_1 is a type (II) matrix. Then we may assume that Y_1 has the form $I_2 \oplus \begin{pmatrix} 0 & y_1 \\ y_2 & 0 \end{pmatrix}$. We claim that $y_1 y_2 = 1$. Otherwise, there are only 32 matrices Z in

$\mathcal{S}_2$ satisfying $(Y_1, Z) = 1$, whereas all the 48 type (III) matrices Z satisfy $(D_1, Z) = 1$. Now, replace ϕ by a mapping of the form $X \mapsto B\phi(X)B$. The modified mapping will satisfy $\phi(D_1) = D_j$ with $j = 3$ or 4. Thus, we are back to case 1.

Case 3. Suppose Y_1 is one of the type (III) matrix. Note that Y_1 cannot have the form PA_jP for $j = 5, 6$, because

$$\min\{(D_1, Z) : Z \in \mathcal{S}_2\} = 0,$$

but for $\{j, k\} = \{5, 6\}$ and we have

$$(PA_jP, PD_1A_kD_1P) = -2$$

and hence

$$\min\{(PA_jP, Z) : Z \in \mathcal{S}_2\} < 0.$$

Now, suppose $Y_1 = PA_jP$ for $j = 1, 2, 3$, or 4. We may assume that $Y_1 = A_j$; otherwise, replace ϕ by $X \mapsto P\phi(X)P$. If $Y_1 = A_1$, replace ϕ by $A \mapsto B\phi(A)B$. The resulting mapping satisfies $\phi(D_1) = E_{11} + E_{23} + E_{32} + E_{44}$. We are back to Case 2.

If $Y_1 = A_2$, A_3 or A_4, replace ϕ by $A \mapsto B\phi(A)B$. The resulting mapping satisfies $\phi(D_1) = E_{11} - E_{23} + E_{32} + E_{44}$, which is impossible by the argument in Case 2. □

4.6 $\mathbf{E}_8$

4.6.1 Matrix realization

The group $\mathbf{E}_8$ has $2^{14}3^5 5^2 7 = 8!2^7 3^3 5$ elements which can be divided into the following 3 classes.

(I) The $8!2^7$ elements of $\mathbf{D}_8$.

(II) The $8!2^{13}$ matrices of the form XAY, where $X, Y \in \mathbf{D}_8$ and

$$A = I_8 - ww^t/4 \qquad \text{with} \qquad w = e - 2e_8 = (1, \cdots, 1, -1)^t \in \mathbf{R}^8. \tag{4.6.15}$$

The counting is done by: $2^7 8!$ choices for each of X and Y, and there are $2 \cdot 8!$ pair of (P, Q) in $\mathbf{D}_8 \times \mathbf{D}_8$ satisfying $PAQ = A$.

(III) The $8!2^8 \cdot 35$ matrices of the form XBY, where $X, Y \in \mathbf{D}_8$ and

$$B = B_1 \oplus B_2 = A(-I_4 \oplus I_4)A, \tag{4.6.16}$$

where

$$B_1 = (1,1,1,1)^t(1,1,1,1)/2 - I_4, \quad B_2 = I_4 - (1,1,1,-1)^t(1,1,1,-1)/2.$$

The counting can be done as follows. First choose 4 rows and 4 columns in $\binom{8}{4}^2$ ways. Then put matrix pairs $(X_1B_1Y_1, X_2B_2Y_2)$ in the two complementary blocks, where

(i) $X_1, Y_1, X_2, Y_2 \in \mathbf{D}_4$,

(ii) $X_1, Y_1, X_2, Y_2 \in (\mathbf{B}_4 \setminus \mathbf{D}_4)$,

(iii) $X_1, X_2 \in \mathbf{D}_4$ and $Y_1, Y_2 \in (\mathbf{B}_4 \setminus \mathbf{D}_4)$, or

(iv) $X_1, X_2 \in (\mathbf{B}_4 \setminus \mathbf{D}_4)$ and $Y_1, Y_2 \in \mathbf{D}_4$.

The number of choices for $X_iB_iY_i$ in each case is $|\mathbf{F}_4 \setminus \mathbf{B}_4|/4 = 4!2^3$. Since $DB_1D = B_2$ with $D = \operatorname{diag}(1,1,1,-1)$, we see that cases (i) and (ii) yield the same matrices, and also cases (iii) and (iv) yield the same matrices. So, there are $2(4!2^3)^2$ so many choices for the pairs. Consequently, the total number of this class is $2(4!2^3)^2\binom{8}{4}^2 = 8!2^7 70$.

4.6.2 Maximum inner product

Let $X \in \mathbf{E}_8$ with $X \neq I$. Then $(I, X) \leq n - 2$. The equality holds if and only if $X = I - (e_i \pm e_j)(e_i \pm e_j)^t$ for some $1 \leq i < j \leq 8$ or $X = P^tAP$ for some $P \in \mathbf{D}_8$. By GP2 in Section 2, for each possible value of $r = (I, X)$, define

$$\mathcal{S}_r = \{X \in \mathbf{E}_8 : (I_8, X) = r\}. \tag{4.6.17}$$

Note that the largest value for r is 6, and $\mathcal{S}_6$ consists of matrices of the following forms.

(a) The 56 matrices of the form

$$X_{ij} = I_8 - (e_i - e_j)(e_i - e_j)^t \qquad \text{or} \qquad Y_{ij} = I_8 - (e_i + e_j)(e_i + e_j)^t,$$

where $1 \leq i < j \leq 8$.

(b) The 64 matrices of the form DAD^t, where A is defined in (4.6.15) and D is a diagonal orthogonal matrix in $\mathbf{D}_8$.

4.6.3 Linear preservers

Theorem 4.5 *A linear operator $\phi : M_8(\mathbf{R}) \to M_8(\mathbf{R})$ satisfies $\phi(\mathbf{E}_8) = \mathbf{E}_8$ if and only if there exist $P, Q \in \mathbf{E}_8$ such that ϕ has the form*

$$X \mapsto PXQ \quad \text{or} \quad X \mapsto PX^tQ.$$

Consequently, $N(\mathbf{E}_8) = \mathbf{E}_8$.

Proof. The assertion on $N(\mathbf{E}_8)$ follows from GP4 in Section 2. The ($\Leftarrow$) part of the first assertion is clear. We consider the ($\Rightarrow$) part. Define $\mathcal{S}_r$ as in (4.6.17).

By Proposition 4.1, if ϕ preserves $\mathbf{E}_8$, then ϕ preserves the inner product $(X,Y) = \mathrm{tr}\,(XY^t)$. By GP3 in Section 2, we may assume that $\phi(I_8) = I_8$ and $\phi(\mathcal{S}_r) = \mathcal{S}_r$ for each r. In the following, we will show that ϕ has the form $X \mapsto P^tXP$ or $X \mapsto P^tX^tP$ for some $P \in \mathbf{E}_8$. We shall use the matrices A, X_{ij} and Y_{ij} as defined in §6.1 – 6.2 as well as the classification of elements of $\mathcal{S}_6$ as type (a) and (b) as defined in §6.2.

Define $D_i = I_8 - 2E_{ii}$, and $D_{ij} = D_iD_j$. Note that those D described in (b) have one of three forms:

$$D_{ij},\ D_{ijkl} = D_{ij}D_{kl}, \qquad \text{or} \qquad -D_{ij}.$$

Note the following four types of conjugations will be used extensively throughout this first part. For i, j, k distinct,

$$X_{ik}X_{jk}X_{ik}^t = X_{ij} \qquad \text{and} \qquad Y_{ik}Y_{jk}Y_{ik}^t = X_{ij}.$$

Since $X_{78} \in \mathcal{S}_6$, it follows that $\phi(X_{78}) = Z \in \mathcal{S}_6$. If $Z = X_{ij}$ or Y_{ij}, then replace ϕ by the mapping $X \mapsto P\phi(X)P^t$ with

$$P = \begin{cases} X_{i7}X_{j8} & \text{if } Z = X_{ij}, \\ X_{i7}Y_{j8} & \text{if } Z = Y_{ij}. \end{cases}$$

Then $\phi(X_{78}) = X_{78}$. If $\phi(X_{78}) = DAD^t$, then replace ϕ by the mapping $X \mapsto D\phi(X)D^t$ so that $\phi(X_{78}) = A$. Furthermore, replace ϕ by the mapping $X \mapsto Q_7\phi(X)Q_7^t$, where $Q_7 = D_{78}AD_{78}^t$, so that $\phi(X_{78}) = X_{78}$.

Now consider those $X \in \mathcal{S}_6$ such that $(X, X_{78}) = 5$. They are of the following two forms.

(c) 24 matrices of the form X_{ij} or Y_{ij} where $i < 7 \le j \le 8$.

(d) 32 matrices of the form DAD^t where $(D, E_{77}) = (D, E_{88}) = 1$.

If $X \in \mathcal{S}_6$ is not of these forms, then $(X, X_{78}) = 4$. It is important to note the sign pattern of the diagonal D in type (d). For any i, j, if $(DAD^t, X_{ij}) = 5$, then (DAD^t, E_{ij}) must be positive. Thus,

$$(D, E_{ii}) = (D, E_{88}) \qquad \text{if } i < j = 8$$

but

$$(D, E_{ii}) = -(D, E_{jj}) \qquad \text{if } i < j < 8.$$

We change the signs in this argument if we are interested in $(DAD^t, X_{ij}) = 4$.

If $\phi(X_{67}) = X_{i7}$ then replace ϕ be the mapping $X \mapsto X_{i6}\phi(X)X_{i6}^t$. If $\phi(X_{67}) = X_{i8}$ then replace ϕ be the mapping $X \mapsto X_{78}\phi(X)X_{78}^t$, thus reducing the problem to the previous case. If $\phi(X_{67}) = Y_{ij}$ then replace ϕ be the mapping $X \mapsto D_{ik}\phi(X)D_{ik}^t$ for $k \neq i, 7, 8$. If $\phi(X_{67}) = DAD^t$ where $(D, E_{77}) = (D, E_{88})$, then replace ϕ be the mapping $X \mapsto \hat{D}\phi(X)\hat{D}^t$ where $\hat{D}$ is a diagonal orthogonal matrix such that $\phi(X_{67}) = Q_7$ where Q_7 is defined as before. Now replace ϕ by the mapping $X \mapsto Q_6\phi(X)Q_6^t$ where $Q_6 = D_{68}AD_{68}^t$ Therefore $\phi(X_{67}) = X_{67}$.

Now consider those $X \in \mathcal{S}_6$ such that $(X, X_{78}) = 4$ and $(X, X_{67}) = 5$. They are of the following two forms.

(e) 10 matrices of the form X_{i6} or Y_{i6}, $i < 6$.

(f) 16 matrices of the form DAD^t where $D = D_{68}$, D_{ij68} or $-D_{ij}$ for $i < j < 6$.

Since X_{56} is in this set, so must $\phi(X_{56})$. If $\phi(X_{56}) = X_{i6}$, then replace ϕ by the mapping $X \mapsto X_{i5}\phi(X)X_{i5}^t$. If $\phi(X_{56}) = Y_{i6}$, then replace ϕ by the mapping

$X \mapsto D_{ik}\phi(X)D_{ik}$ where $k < 6$. If $\phi(X_{56}) = DAD^t$ where $(D, E_{66}) = -(D, E_{77}) = (D, E_{88})$, then replace ϕ by the mapping $X \mapsto \hat{D}\phi(X)\hat{D}^t$ where $\hat{D} = DD_{68}$. Next replace ϕ by the mapping $X \mapsto Q_5\phi(X)Q_5^t$ where $Q_5 = D_{58}AD_{58}^t$.

We can fix first, X_{45}, second, X_{34}, and third, X_{23}, in the same way as we fixed X_{56} by the following arguments. For $k = 5$, 4 and then 3, consider those $X \in \mathcal{S}_6$ that have inner product of 5 with the matrix $X_{k,k+1}$ (which has just been shown to be fixed by ϕ) but inner product of 4 with $X_{i,i+1}$ for $i \geq k+1$. Then $\phi(X_{k-1,k})$ have one of three forms: $X_{i,k-1}$, $Y_{i,k-1}$ and DAD where $D = \hat{D}D_{k-1,8}$. If it is one of the first two forms, then replace ϕ by a mapping of the form $X \mapsto P\phi(X)P^t$ where P is a appropriate matrix of one of the first two forms. If it is of the third form, replace ϕ by the mapping

$$X \mapsto Q_{k-1}\hat{D}\phi(X)\hat{D}Q_{k-1} \qquad \text{for} \qquad Q_{k-1} = D_{k-1,8}AD_{k-1,8}.$$

Now define $Q_1 = D_{18}AD_{18}^t$. Then Q_1 is the only type (b) matrix such that $Q_1 \in \mathcal{S}_6$ and $(Q_1, X_{i,i+1}) = 4$ for $i = 2, ..., 7$. There are no type (a) matrices where this property holds, thus $\phi(Q_1) = Q_1$. Consider those $X \in \mathcal{S}_6$ such that $(X, X_{23}) = 5$ and $(X, X_{i,i+1}) = 4$ for $i = 3, ..., 7$. Then $X = X_{12}$, Y_{12} or Q_2. Inspecting the sign pattern, we have $(X_{ij}, Q_1) \neq (Y_{ij}, Q_1)$ for all i, j. Thus, we may assume that $\phi(X_{12}) = X_{12}$. Otherwise $\phi(X_{12}) = Q_2$ and replace ϕ by the mapping $X \mapsto Q_1\phi(X)Q_1$. Thus, $\phi(Z) = Z$ for $Z = I_8, Q_1, X_{i,i+1}$ for $i = 1, ..., 7$. One can check that this is sufficient to show that $\phi(X) = X$ for all $X \in \mathcal{S}_6$; see the last section.

Suppose that $\phi(X) = Y$ for some $X \in \mathbf{E}_8$. Then

$$2(X, E_{ij} + E_{ji}) = (X, X_{ij} - Y_{ij}) = (Y, X_{ij} - Y_{ij}) = 2(Y, E_{ij} + E_{ji}).$$

Also, for all $i \neq j$, $I - (X_{ij} + Y_{ij})/2 = E_{ii} + E_{jj}$. Therefore, $(X, E_{ii}) = (Y, E_{ii})$ for all i and thus

$$\phi(X) = X \text{ or } X^t \qquad \text{for all } X \in \mathbf{E}_8.$$

Let $X_{ijk} = X_{ij}X_{ik} \in \mathcal{S}_5$ for each $i < j < k$. Then X_{ijk} is the type (I) matrix with the following principal submatrices

$$X_{ijk}(i, j, k) = I_5, \qquad X_{ijk}[i, j, k] = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}.$$

Here $Z[i, j, k]$ denotes the submatrix of Z lying in rows and columns i, j, and k; and $Z(i, j, k)$ denotes the matrix obtained from Z by deleting its rows and columns indexed by i, j, and k. Then we may assume that $\phi(X_{678}) = X_{678}$. Otherwise, $\phi(X_{678}) = X_{678}^t$, and replace ϕ by the mapping $X \mapsto \phi(X)^t$. Note that $(X_{ijk}, X_{678}) = 5$ if and only if $i < 6 \leq j < k \leq 8$. But then $(X_{ijk}^t, X_{678}) = 4$. Thus $\phi(X_{ijk}) = X_{ijk}$ for all X_{ijk} where $i < 6 \leq j < k \leq 8$. Continuing in this manner, we can fix all matrices of the form X_{ijk}. Therefore $\phi(Z) = Z$ whenever X_{ijk} for all $1 \leq i < j < k \leq 8$.

Let

$$P = E_{1n} + \sum_{j=2}^{n} E_{j,j-1} \in M_8(\mathbf{R}).$$

Then, for all $Q \in \mathcal{S}_6$ of type (b), $\phi(PQ) = PQ$ or $(PQ)^t$. But clearly, $(PQ, X_{123}) \neq ((PQ)^t, X_{123})$, therefore, $\phi(PQ) = PQ$ for all $Q \in \mathcal{S}_6$ of type (b). Thus, $\phi(Z) = Z$

for $Z = I_8, X_{ijk}$ where $i < j < k$, X_{ij} where $i < j$ and for $Z = Q$ and PQ for all $Q \in \mathcal{S}_6$ of type (b). One can check that these matrices span $M_8(\mathbf{R})$; see the last section. Thus $\phi(X) = X$ for all $X \in \mathbf{E}_8$. □

4.7 $\mathbf{E}_7$

Let

$$w = e - 2e_8 \in \mathbf{R}^8.$$

Then $\mathbf{E}_7$ has a natural realization as a subgroup of $\mathbf{E}_8 \subseteq M_8$ defined and denoted by

$$\mathcal{E}_7 = \{X \in \mathbf{E}_8 : Xw = w\}$$

acting on the 7-dimensional subspace $w^\perp$ in $\mathbf{R}^8$. Suppose U is an orthogonal matrix with $w/\sqrt{8}$ as the first column. Then for every $A \in \mathcal{E}_7$, we have

$$U^tAU = \begin{pmatrix} 1 & 0 \\ 0 & \hat{A} \end{pmatrix}. \tag{4.7.18}$$

The collection of such $\hat{A} \in M_7(\mathbf{R})$ will form a matrix realization of $\mathbf{E}_7$ in $M_7(\mathbf{R})$. Moreover, for any $A, B \in \mathcal{E}_7$ and the corresponding $\hat{A}, \hat{B} \in \mathbf{E}_7$, we have

$$(A, B) = \operatorname{tr}(AB^t) = 1 + \operatorname{tr}(\hat{A}\hat{B}^t) = 1 + (\hat{A}, \hat{B}). \tag{4.7.19}$$

Of course, one may have different realizations of $\mathbf{E}_7$ in $M_7(\mathbf{R})$ by a different choice of U. Nonetheless, it is well known that all the realizations of $\mathbf{E}_7$ in $O(7)$ are orthogonally similar. In this section, we will study $\mathbf{E}_7$ via $\mathcal{E}_7$ as mentioned in GP5 of section 2.

4.7.1 Matrix realization

The group $\mathcal{E}_7 = \{X \in \mathbf{E}_8 : Xw = w\}$ has 8!72 elements which can be divided into the following three classes.

(I) The 8! elements in $\mathbf{D}_8 \cap \mathcal{E}_7$, those elements $X \in \mathbf{D}_8$ such that $Xw = w$.

(II) The 8!36 matrices of the form X^tAY satisfying $X^tAYw = w$, where $X, Y \in \mathbf{D}_8$ and $A = I_8 - ww^t/4$ with $w = e - 2e_8 = (1, \cdots, 1, -1)^t \in \mathbf{R}^8$. The counting is done as follows. Consider the equation $AYw = Xw$, i.e., $Yw - Xw = w(w^tYw)/4$. There are 3 cases.

(i) $w^tYw = 8$, $Yw - Xw = 2w$. Then $Yw = w = -Xw$. There are 8! choices for each of X and Y and there are 8! pairs (P, Q) in $\mathbf{D}_8 \times \mathbf{D}_8$ such that $PAQ = A$ with $Qw = w$ and $w^tP = w^t$. So, there are 8! elements in this case. Clearly, these must coincide with the 8! elements of the form $-PA$ where P is a matrix of type (I).

(ii) $w^tYw = -8$, $Yw - Xw = -2w$. Then $Yw = -w = -Xw$. Every pair (X, Y) in (b.i) can be converted to $(-X, -Y)$ to this case, and we actually get the same $XAY = (-X)A(-Y)$ matrix. So, no new addition in this case.

(iii) $w^tYw = 0$, $Yw = Xw$. For each of the 70 choices of $w_i \in w^\perp$, where all entries of w_i are ± 1, we have a fixed $P_i \in \mathbf{D}_8$ such that $P_iw = w_i$, $Y = P_i\hat{Y}$ and $X = P_i\hat{X}$ with $\hat{Y}w = w = \hat{X}w$. Now, there are 8! choices for each of $\hat{X}$ and $\hat{Y}$, and we have to factor out the 8! so many (R, S) pairs such that $R^t(P_i^tAP_i)S = P_i^tAP_i$ with $Sw = w = Rw$. Thus, there are 8! so many X^tAY corresponding to each choice of w_i. However, for each w_i, the 8! matrices X^tAY corresponding to w_i are the same as the 8! matrices corresponding to $-w_i$. Thus, we have $8!70/2 = 8!35$ matrices in this case. These are the matrices of the form $PDAD^t$ where P is a type (I) matrix and D is a diagonal matrix whose diagonal entries are permutations of $(1,1,1,1,-1,-1,-1,-1)$. In other words, $Dw \in w^{\perp}$.

(III) The 8!35 matrices of the form X^tBY satisfying $X^tBYw = w$, where $X, Y \in \mathbf{D}_8$ and $B = B_1 \oplus B_2 = A(-I_4 \oplus I_4)A$, where

$$B_1 = (1,1,1,1)^t(1,1,1,1)/2 - I_4, \quad B_2 = I_4 - (1,1,1,-1)^t(1,1,1,-1)/2.$$

The counting is done as follows. In order to have $X^tBYw = w$, the last row of X^tBY must contain either a row of $X_2B_2Y_2$ with a nonzero $(8,8)$ entry or a row of $X_1B_1Y_1$ with the $(8,8)$ equal to zero. In the first case, we have $\binom{7}{4}\binom{7}{4}4!$ ways to put $X_1B_1Y_1$ so as to make the first 4 entries of X^tBYw equal to 1, and then 4! ways to put the $X_2B_2Y_2$ matrices so that the last 4 entries of X^tBYw are $1,1,1,-1$. In the second case, we have $\binom{7}{4}\binom{7}{4}4!$ ways to put $X_2B_2Y_2$ so as to make the first 4 entries of X^tBYw equal to 1, and then 4! ways to put the $X_1B_1Y_1$ matrices so that the last 4 entries of X^tBYw are $1,1,1,-1$. Thus, total number is $2(\binom{7}{4}\binom{7}{4}(4!)^2) = 8!35$.

4.7.2 Maximum inner product

Let $X \in \mathcal{E}_7$ with $X \neq I$. Then $(I_8, X) \leq 6$ and hence the inner product on the irreducible subspace $\mathbf{E}_7$ is bounded by 5. Using the matrix realization in $M_8(\mathbf{R})$ and by GP2 in Section 2, for each possible value of $r = (I_8, X)$, define

$$\mathcal{S}_r = \{X \in \mathcal{E}_7 : (I_8, X) = r\}. \tag{4.7.20}$$

Note that $\mathcal{S}_6$ consists of matrices in one of the following two forms.

(a) The 28 matrices X_{ij} of the form

$$X_{ij} = I_8 - (e_i - e_j)(e_i - e_j)^t \text{ for } 1 \leq i < j \leq 7$$

$$X_{i8} = I_8 - (e_i + e_8)(e_i + e_8)^t \text{ for } 1 \leq i \leq 7.$$

(b) The 35 matrices of the form $X = DAD^t$ for some diagonal orthogonal D such that $Dw \in w^\perp$.

4.7.3 Linear preservers

Theorem 4.6 *A linear operator $\psi : M_7(\mathbf{R}) \to M_7(\mathbf{R})$ satisfies $\psi(\mathbf{E}_7) = \mathbf{E}_7$ if and only if there exist $P, Q \in \mathbf{E}_7$ such that ψ has the form*

$$X \mapsto PXQ \quad or \quad X \mapsto PX^tQ.$$

Consequently, $N(\mathbf{E}_7) = \mathbf{E}_7$.

Proof. The assertion on $N(\mathbf{E}_7)$ follows from GP4 in Section 2. The ($\Leftarrow$) part of the first assertion is clear. We consider the ($\Rightarrow$) part. Let $\psi : M_7(\mathbf{R}) \to M_7(\mathbf{R})$ be a linear map satisfying $\psi(\mathbf{E}_7) = \mathbf{E}_7$. By Proposition 4.1, if ψ preserves $\mathbf{E}_7$, then ψ preserves the inner product $(\hat{X}, \hat{Y}) = \operatorname{tr}(\hat{X}\hat{Y}^t)$. Also, by GP3 in Section 2, we may assume that $\psi(I_7) = I_7$.

Let V_7 be the affine space generated by $\mathcal{E}_7$, and let U be an orthogonal matrix establishing the correspondence between $\mathcal{E}_7$ and $\mathbf{E}_7$ as described in (4.7.18). Consider an affine map $\phi : V_7 \to V_7$ defined by

$$\phi\left(U\begin{pmatrix}1 & 0\\ 0 & \hat{X}\end{pmatrix}U^t\right) = U\begin{pmatrix}0 & 0\\ 0 & \psi(\hat{X})\end{pmatrix}U^t + U\begin{pmatrix}1 & 0\\ 0 & 0_7\end{pmatrix}U^t.$$

Then $\phi(\mathcal{E}_7) = \mathcal{E}_7$. Since ψ preserves inner product in $M_7(\mathbf{R})$, we have $(\phi(X), \phi(Y)) = (X, Y)$ for all $X, Y \in \mathcal{E}_7$ by (4.7.19). Define $\mathcal{S}_r$ as in (4.7.20). Since $\psi(I_7) = I_7$, therefore, $\phi(I_8) = I_8$ and by GP3 in Section 2, $\phi(\mathcal{S}_r) = \mathcal{S}_r$ for each r. In the following, we will show that for some $P \in \mathcal{E}_7$, ϕ has the form

$$X \mapsto P^t X P \text{ for all } X \in \mathcal{E}_7 \qquad \text{or} \qquad X \mapsto P^t X^t P \text{ for all } X \in \mathcal{E}_7.$$

We shall use the matrices A and X_{ij} for $1 \leq i < j \leq 8$ as defined in §7.1–7.2. We also refer to matrices in $\mathcal{S}_6$ as type (a) and (b) matrices as defined in §7.2. Furthermore, let $D_i = I_8 - 2E_{ii}$, and $D_{ij} = D_i D_j$. Note that those D described in (b) will be of the form $D_{ijkl} = D_{ij} D_{kl}$ where i, j, k, l are all distinct. If i', j', k', l' are such that $\{i, i', j, j', k, k', l, l'\} = \{1, ..., 8\}$, then

$$D_{ijkl} A D_{ijkl} = D_{i'j'k'l'} A D_{i'j'k'l'}.$$

Also, for i, j, k distinct and X_{jk}, X_{ik} and X_{ij} all of type (a),

$$X_{ik} X_{jk} X_{ik}^t = X_{ij}.$$

We may assume that $\phi(X_{78}) = X_{78}$. Otherwise $\phi(X_{78}) = X_{ij}$ or $\phi(X_{78}) = DAD$ for an appropriate D. If $\phi(X_{78}) = X_{ij}$, then replace ϕ by the mapping $X \mapsto P\phi(X)P^t$ where P is an appropriate type (a) matrix. If $\phi(X_{78}) = DAD^t$, then consider D. If $D = D_{ijk7}$ for $i, j, k < 7$, then replace ϕ by the mapping $X \mapsto QAQ^t$ where $Q = D_{ijk8} A D_{ijk8}$. If $D = D_{ij78}$, Then replace ϕ by the mapping $X \mapsto X_{k8}\phi(X)X_{k8}^t$ for some $k \neq i, j$. Thus $\phi(X_{78}) = D_{ijk7} A D_{ijk7}$, which has already been discussed. Therefore, $\phi(X_{78}) = X_{78}$.

Now, consider those $X \in S_6$ such that $(X, X_{78}) = 5$. They are of two forms.

(c) 12 matrices of the form X_{ij} for $i < 7 \leq j$.

(d) 20 matrices of the form DAD where $D = D_{ijk7}$ and $i < j < k < 7$.

We may assume that $\phi(X_{67}) = X_{67}$. Otherwise $\phi(X_{67}) = X_{ij}$ where $i < 6$ and $7 \leq j$ or $\phi(X_{67}) = DAD$ where $D = D_{ijk7}$ and $i < j < k < 7$. If $\phi(X_{67}) = X_{i7}$ where $i < 6$ then replace ϕ by the mapping $X \mapsto X_{i6}\phi(X)X_{i6}^t$. If $\phi(X_{67}) = X_{i8}$ where $i < 6$, then replace ϕ by the mapping $X \mapsto X_{78}\phi(X)X_{78}^t$ and we are back to the previous case. If $\phi(X_{67}) = DAD$ where $D = D_{ijk7}$ and $i < j < k < 7$, then either $k = 6$ or $k \neq 6$. If $k \neq 6$, then replace ϕ by the mapping of the form $X \mapsto QAQ^t$ where $Q = D_{ijk6}AD_{ijk6}$. If $k = 6$, replace ϕ by the mapping $X \mapsto X_{k'6}\phi(X)X_{k'6}$ where $k' \neq i, j$ and also $k' < 6$. Therefore, $\phi(X_{67}) = X_{67}$.

Now, consider those $X \in S_6$ such that $(X, X_{78}) = 4$ and $(X, X_{67}) = 5$. They are of two forms.

(e) 5 matrices of the form X_{i6} for $i < 6$.

(f) 10 matrices of the form DAD where $D = D_{ijk6}$ and $i < j < k < 6$.

We may assume that $\phi(X_{56}) = X_{56}$. Otherwise $\phi(X_{56}) = X_{i6}$ where $i < 5$ or $\phi(X_{56}) = DAD$ where $D = D_{ijk6}$ and $i < j < k < 6$. If $\phi(X_{56}) = X_{i6}$ where $i < 5$ then replace ϕ by the mapping $X \mapsto X_{i5}\phi(X)X_{i5}^t$. If $\phi(X_{56}) = DAD$ where $D = D_{ijk6}$ and $i < j < k < 6$, then either $k = 5$ or $k \neq 5$. If $k \neq 5$, then replace ϕ by the mapping of the form $X \mapsto QAQ^t$ where $Q = D_{ijk5}AD_{ijk5}$. If $k = 5$, replace ϕ by the mapping $X \mapsto X_{k'5}\phi(X)X_{k'5}$ where $k' \neq i, j$ and also $k' < 5$. Therefore,

$\phi(X_{56}) = X_{56}$. We may also fix X_{45} in a similar manner, using those $X \in \mathcal{S}_6$ such that $(X, X_{56}) = 5$, but has inner product 4 with the other fixed matrices.

Now, consider those $X \in \mathcal{S}_6$ such that

$$[(X, X_{78}), (X, X_{67}), (X, X_{56}), (X, X_{45})] = [4, 4, 4, 4].$$

Then $X = X_{12}, X_{13}$ or X_{23}. We may assume that $\phi(X_{12}) = X_{12}$. Otherwise $\phi(X_{12}) = X_{i3}$ for $i = 1$ or 2, in which case, replace ϕ by the mapping $X \mapsto X_{j3}\phi(X)X_{j3}$ where $\{i, j\} = \{1, 2\}$. We may also assume that $\phi(X_{23}) = X_{23}$; otherwise $\phi(X_{23}) = X_{13}$. If this is the case, replace ϕ by the mapping $X \mapsto X_{12}\phi(X)X_{12}$. Thus $\phi(Z) = Z$ for

$$Z = X_{12}, X_{23}, X_{45}, X_{56}, X_{67} \text{ and } X_{78}.$$

One can check that this requires that $\phi(X) = X$ for all $X \in \mathcal{S}_6$; see the last section.

Consider those $X \in \mathcal{E}_7$ such that $X_{ij}X \in \mathcal{S}_6$ and $(X_{ij}X, X_{ij}) = 5$. In other words, $X \in \mathcal{S}_5$ and $(X, X_{ij}) = 6$. So X is of the form $X_{ij}X_{lk}$, where $k \notin \{i, j\}$ but $l \in \{i, j\}$, or the form $X_{ij}DAD^t$ where $Dw \in w^{\perp}$ and $(D, E_{ii}) = -(D, E_{jj})$. If we add the condition that $(X, X_{ik}) = 6$ and $(X, X_{jk}) = 6$, then X must be of the form $X_{ij}X_{ik}$ or $X_{ij}X_{jk} = (X_{ij}X_{ik})^t$. Let $X_{ijk} = X_{ij}X_{ik} \in \mathcal{S}_5$ for each $i < j < k$. Then X_{ijk} is the type (I) matrix with the following principal submatrices.

$$X_{ijk}(i, j, k) = I_5, \qquad X_{ijk}[i, j, k] = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & \epsilon_1 \\ \epsilon_2 & 0 & 0 \end{pmatrix},$$

where $\epsilon_1 = \epsilon_2 = 1$ if $k < 8$ and -1 if $k = 8$. Thus, $\phi(X_{ijk}) = X_{ijk}$ or $\phi(X_{ijk}) = X_{ijk}^t$ for all $i < j < k$. Then we may assume that $\phi(X_{678}) = X_{678}$. Otherwise, $\phi(X_{678}) = X_{678}^t$

and replace ϕ by the mapping $X \mapsto \phi(X)^t$. Thus, also $\phi(X_{678}^t) = X_{678}^t$. Consider those X_{ijk} such that $(X_{ijk}, X_{678}) = 5$. Then either $\{j,k\} = \{6,7\}$ or $\{j,k\} = \{7,8\}$. But for those X_{ijk}, $(X_{ijk}, X_{678}^t) = 4$. So $\phi(X_{ijk}) = X_{ijk}$ for all such X_{ijk}. Using these newly fixed matrices, continue in the same manner until $\phi(X_{ijk}) = X_{ijk}$ for all X_{ijk} such that $1 \leq i < j < k \leq 8$.

We have shown that $\phi(X) = X$ for all $X \in \mathcal{S}_6$, $X = I_8$ and all X of the form X_{ijk}. It can be shown (see the last section) that there are 50 linearly independent matrices in this collection. Given this, and the fact that

$$\phi(0) = U \begin{pmatrix} 1 & 0 \\ 0 & 0_7 \end{pmatrix} U^t,$$

we see that the linear map

$$\phi(X) - \phi(0)$$

is completely determined. In particular, $\phi(X) = X$ for all $X \in \mathcal{E}_7$. It follows that the original affine map ϕ on V_7 has the form

$$X \mapsto P^t X P \qquad \text{or} \qquad X \mapsto P^t X^t P$$

for some $P \in \mathcal{E}_7$. Note that if $P, X \in \mathcal{E}_7$, there exists $\hat{P}, \hat{X} \in \mathbf{E}_7$ such that

$$P^t X P = U \begin{pmatrix} 0 & 0 \\ 0 & \hat{P}^t \hat{X} \hat{P} \end{pmatrix} U^t + U \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} U^t.$$

Thus, there exists a $\hat{P} \in \mathbf{E}_7$ such that

$$\psi(\hat{X}) = \hat{P}^t \hat{X} \hat{P} \text{ for all } \hat{X} \in \mathbf{E}_7 \qquad \text{or} \qquad \psi(\hat{X}) = \hat{P}^t \hat{X}^t \hat{P} \text{ for all } \hat{X} \in \mathbf{E}_7.$$

Since $\mathbf{E}_7$ spans $M_7(\mathbf{R})$, ψ on $M_7(\mathbf{R})$ has the asserted form. $\square$

Note that in the above proof, we showed that an affine map ϕ on V_7 satisfies $\phi(\mathcal{E}_7) = \mathcal{E}_7$ and preserves the inner product on V_7 if and only if there exists $P, Q \in \mathcal{E}_7$ such that ϕ has the form

$$X \mapsto PXQ \qquad \text{or} \qquad X \mapsto PX^tQ \tag{4.7.21}$$

on V_7. The same proof can actually be used to show that a linear map $\hat{\phi}$: span $\mathcal{E}_7 \mapsto$ span $\mathcal{E}_7$ satisfies $\hat{\phi}(\mathcal{E}_7) = \mathcal{E}_7$ and preserves the inner product on span $\mathcal{E}_7$ if and only if there exists $P, Q \in \mathcal{E}_7$ such that $\hat{\phi}$ has the form (4.7.21).

4.8 $\mathbf{E}_6$

In this section, continue to write

$$w = e - 2e_8 \in \mathbf{R}^8$$

and let

$$v = e_7 - e_8 \in \mathbf{R}^8.$$

Then $\mathbf{E}_6$ has a natural realization as a subgroup of $\mathbf{E}_8 \subseteq M_8$ defined and denoted by

$$\mathcal{E}_6 = \{X \in \mathcal{E}_7 : Xv = v\} = \{X \in \mathbf{E}_8 : Xv = v \text{ and } Xw = w\}$$

acting on the 6-dimensional subspace span $(v, w)^{\perp}$ in $\mathbf{R}^8$. Suppose U is an orthogonal matrix with $w/\sqrt{8}$ as the first column and the normalization of the component of v orthogonal to w as the second column. Then for every $A \in \mathcal{E}_6$, we have

$$U^tAU = \begin{pmatrix} I_2 & 0 \\ 0 & \hat{A} \end{pmatrix}. \tag{4.8.22}$$

The collection of such $\hat{A} \in M_6(\mathbf{R})$ will form a matrix realization of $\mathbf{E}_6$ in $M_6(\mathbf{R})$. Moreover, for any $A, B \in \mathcal{E}_6$ and the corresponding $\hat{A}, \hat{B} \in \mathbf{E}_6$, we have

$$(A, B) = \operatorname{tr}(AB^t) = 2 + \operatorname{tr}(\hat{A}\hat{B}^t) = 2 + (\hat{A}, \hat{B}). \tag{4.8.23}$$

Of course, one may have different realizations of $\mathbf{E}_6$ in $M_6(\mathbf{R})$ by a different choice of U. Nonetheless, it is well known that all the realizations of $\mathbf{E}_6$ in $O(6)$ are orthogonally similar. In this section, we will study $\mathbf{E}_6$ via $\mathcal{E}_6$ as mentioned in GP5 of section 2.

4.8.1 Matrix realization

The group $\mathcal{E}_6 = \{X \in \mathbf{E}_8 : Xw = w,\ Xv = v\}$ has 6!72 elements which can be divided into the following 3 classes of matrices arising from $\mathcal{E}_7$.

(I) The 6!2! elements in $\mathbf{D}_8 \cap \mathbf{E}_6$, namely, those elements $X \in \mathbf{D}_8$ of the form $X = X_1 \oplus X_2$ for suitable choices of $X_1 \in \mathbf{B}_6$ and

$$X_2 = I_2 \qquad \text{or} \qquad X_2 = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}.$$

(II) The 6!40 matrices of the form X^tAY satisfying $X^tAYw = w$ and $X^tAYv = v$, where $X, Y \in \mathbf{D}_8$ and $A = I_8 - ww^t/4$ with $w = e - 2e_8 = (1, \cdots, 1, -1)^t \in \mathbf{R}^8$. The counting is done as follows. Consider the equations $AYw = Xw$ and $AYv = Xv$, i.e.,

$$Yw - Xw = w(w^tYw)/4 \text{ and } Yv - Xv = w(w^tYv)/4.$$

Clearly, we must have $w^tYv = 0$. Thus, we are studying the (II.iii) matrices of $\mathcal{E}_7$ in §7.1. First, if $w_i \in \{w, v\}^\perp$ such that all entries of w_i are ± 1, then the last two entries of w_i have the same sign, and 3 of the first six entries equal to 1. So, there are $2 \cdot \binom{6}{3} = 40$ possibilities. For each of the 40 choices of $w_i \in \{w, v\}^{\perp}$, where all entries of w_i are ± 1, we have a fixed $P_i \in \mathbf{D}_8$ such that $P_i w = w_i$, $Y = P_i \hat{Y}$. There are 8! choices of such $\hat{Y}$, and for a fixed $\hat{Y}$ there are 6!2! choices of $\hat{X} \in \mathbf{D}_8$ so that $\hat{X} w = w$ and $P\hat{X} v = P\hat{Y} v$. We have to factor out the 8! so many (R, S) pairs such that $R(P_i^t A P_i)S = P_i^t A P_i$ with $Sw = w = R^t w$. Thus, there are 6!2! so many $X^t A Y$ corresponding to each choice of w_i. However, for each w_i, the 6!2! matrices $X^t A Y$ are the same as those corresponding to $-w_i$. Thus, we have $20(6!2!) = 6!40$ matrices of $\mathbf{E}_6$ in this class. And we also see that they are equivalent to matrices of the form $YDAD$ where Y is a matrix of type (I) and D is a diagonal orthogonal matrix such that $Dw \in w^{\perp}$ and $(D, E_{77}) = -(D, E_{88})$.

(III) The 6!30 matrices of the form $X^t B Y$ satisfying $X^t B Y w = w$ and $X^t B Y v = v$, where $X, Y \in \mathbf{D}_8$ and $B = B_1 \oplus B_2 = A(-I_4 \oplus I_4)A$, where

$$B_1 = (1,1,1,1)^t(1,1,1,1)/2 - I_4, \quad B_2 = I_4 - (1,1,1,-1)^t(1,1,1,-1)/2.$$

The counting is done as follows. In order to have $X^t B Y w = w$ and $X^t B Y v = v$, the 2×2 submatrix of $X^t B Y$ at the right bottom corner cannot contain zero entries. Thus, we have to choose from the first 6 rows and the first 6 columns a 4×4 submatrix to accommodate an $X_1 B_1 Y_1$ as described in $\mathbf{E}_7$, and there are $\binom{6}{4}^2 4!$ ways and there are 4 ways to fixed the matrix $X_2 B_2 Y_2$. Thus there are $\binom{6}{4}^2 4! 4 = 6!30$ matrices in this case.

4.8.2 Maximum inner product

Let $X \in \mathcal{E}_6$ with $X \neq I_8$. Then $(I_8, X) \leq 6$. Therefore the inner product on the irreducible subspace $\mathbf{E}_6$ is bounded by 4. Using the matrix realization in $M_8(\mathbf{R})$ and by GP2 in Section 2, for each possible value of $r = (I_8, X)$, define

$$\mathcal{S}_r = \{X \in \mathcal{E}_6 : (I_8, X) = r\}. \tag{4.8.24}$$

Note that $\mathcal{S}_6$ consists of matrices in one of the following two forms.

(a) The 16 matrices of the form $X_{ij} = I_8 - (e_i - e_j)(e_i - e_j)^t$ for some $1 \leq i < j \leq 6$ and $X_{78} = I_8 - (e_7 + e_8)(e_7 + e_8)^t$.

(b) The 20 matrices of the form $X = DAD$ where D is an orthogonal diagonal matrix such that $Dw \in w^\perp$ and $(D, E_{77}) = -(D, E_{88})$.

4.8.3 Linear preservers

Theorem 4.7 *A linear operator $\psi : M_6(\mathbf{R}) \to M_6(\mathbf{R})$ satisfies $\psi(\mathbf{E}_6) = \mathbf{E}_6$ if and only if there exist $P, Q \in \mathbf{E}_6$ such that ψ has the form*

$$X \mapsto PXQ \quad \text{or} \quad X \mapsto PX^tQ.$$

Consequently, $N(\mathbf{E}_6) = \mathbf{E}_6$.

Proof. The assertion on $N(\mathbf{E}_6)$ follows from GP4 in Section 2. The $(\Leftarrow)$ part of the first assertion is clear. We consider the $(\Rightarrow)$ part. Let $\psi : M_6(\mathbf{R}) \to M_6(\mathbf{R})$ be a linear map satisfying $\psi(\mathbf{E}_6) = \mathbf{E}_6$. By Proposition 4.1, if ψ preserves $\mathbf{E}_6$, then ψ

preserves the inner product $(\hat{X},\hat{Y}) = \mathrm{tr}\,(\hat{X}\hat{Y}^t)$ on $M_6(\mathbf{R})$. Also, by GP3 in Section 2, we may assume that $\psi(I_6) = I_6$.

Let V_6 be the affine space generated by $\mathcal{E}_6$, and let U be an orthogonal matrix establishing the correspondence between $\mathcal{E}_6$ and $\mathbf{E}_6$ as described in (4.8.22). Consider an affine map $\phi : V_6 \to V_6$ defined by

$$\phi\left(U\begin{pmatrix} I_2 & 0 \\ 0 & \hat{X}\end{pmatrix}U^t\right) = U\begin{pmatrix} 0_2 & 0 \\ 0 & \psi(\hat{X})\end{pmatrix}U^t + U\begin{pmatrix} I_2 & 0 \\ 0 & 0_6\end{pmatrix}U^t.$$

Then $\phi(\mathcal{E}_6) = \mathcal{E}_6$. Since ψ preserves inner product in $M_6(\mathbf{R})$, we have $(\phi(X),\phi(Y)) = (X,Y)$ for all $X, Y \in \mathcal{E}_6$ by (4.8.23). Define $\mathcal{S}_r$ as in (4.8.24). Since $\psi(I_6) = I_6$, therefore, $\phi(I_8) = I_8$ and by GP3 in Section 2, $\phi(\mathcal{S}_r) = \mathcal{S}_r$ for each r. In the following, we will show that for some $P \in \mathcal{E}_6$, ϕ has the form

$$X \mapsto P^tXP \text{ for all } X \in \mathcal{E}_6 \qquad \text{or} \qquad X \mapsto P^tX^tP \text{ for all } X \in \mathcal{E}_6.$$

We shall use the matrices A and X_{ij} as defined in §8.1 – 8.2. Also, we shall use the classification of matrices in $\mathcal{S}_6$ into types (a) and (b) as defined in §8.2.

Define $D_i = I_8 - 2E_{ii}$, and $D_{ij} = D_iD_j$. Note that those D described in (b) will be of the form $D_{ijk7} = D_{ij}D_{k7}$ where $i, j, k \neq 7$ are all distinct. If i', j', k' are such that $\{i, i', j, j', k, k'\} = \{1, ..., 6\}$, then

$$D_{ijk7}AD_{ijk7} = D_{i'j'k'8}AD_{i'j'k'8}.$$

Also, for i, j, k distinct, $i, j, k < 7$ and X_{jk}, X_{ik} and X_{ij} all of type (a),

$$X_{ik}X_{jk}X_{ik}^t = X_{ij}.$$

Let $\phi(X_{78}) = Z$. If $Z = X_{78}$ then we are done. If $Z = DAD$, where $D = D_{ijk7}$, then replace ϕ by the mapping $X \mapsto Q\phi(X)Q^t$ where $Q = D_{ijk8}AD_{ijk8}$. And so $\phi(X_{78}) = X_{78}$. If, on the other hand, $Z = X_{ij}$ for $i < j < 7$, then replace ϕ by the mapping $X \mapsto Q\phi(X)Q^t$ where $Q = D_{ikl7}AD_{ikl7}$ for $k, l \neq i, j, 7, 8$. Thus $\phi(X_{87}) = DAD$ where $D = D_{jkl7}$, and this case has already been covered. Therefore, $\phi(X_{78}) = X_{78}$.

Note that if $X \in \mathcal{S}_6$ is of type (a), then $(X, X_{78}) = 4$, while if X is of type (b), then $(X, X_{78}) = 5$. Thus, those $X \in \mathcal{S}_6$ that are of type (a) are mapped to themselves, and those of type (b) are mapped to themselves.

We may assume that $\phi(X_{56}) = X_{56}$. Otherwise, $\phi(X_{56}) = X_{ij}$ where $(i, j) \neq (5, 6)$ and $i < j \leq 6$. Then replace ϕ by the mapping $X \mapsto P\phi(X)P^t$ where

$$P = \begin{cases} X_{i5} & \text{if } j = 6, \\ X_{i6} & \text{if } j = 5, \\ X_{i5}X_{i6} & \text{if } i < j < 5. \end{cases}$$

Now consider those $X \in \mathcal{S}_6$ of type (a) such that $(X, X_{56}) = 5$. Then $X = X_{ij}$ where $i < j$ and $j \in \{5, 6\}$. We may assume that $\phi(X_{45}) = X_{45}$. Otherwise $\phi(X_{45}) = X_{ij}$ where $j \in \{5, 6\}$. If $j = 5$, then replace ϕ by the mapping $X \mapsto X_{i4}\phi(X)X_{i4}$. If $j = 6$, then replace ϕ by the mapping $X \mapsto X_{56}\phi(X)X_{56}$ and so we are back to the case where $j = 5$.

Now consider those $X \in \mathcal{S}_6$ of type (a) such that $(X, X_{56}) = 4$ and $(X, X_{45}) = 5$. They must be of the form X_{i4}. We may assume that $\phi(X_{34}) = X_{34}$. Otherwise it equals X_{i4} for $i \in \{1, 2\}$, in which case, replace ϕ by the mapping $X \mapsto X_{i3}\phi(X)X_{i3}$.

Now consider those $X \in \mathcal{S}_6$ of type (a) such that $(X, X_{56}) = 4$, $(X, X_{45}) = 4$ and $(X, X_{34}) = 5$. Then $X = X_{13}$ or X_{23}. If $\phi(X_{23}) = X_{13}$, then replace ϕ by the mapping $X \mapsto X_{12}\phi(X)X_{12}$. And thus, $\phi(X_{23}) = X_{23}$. By considering the inner products, we also see that $\phi(X_{12}) = X_{12}$. Thus $\phi(Z) = Z$ for $Z = I_8$, X_{78}, X_{56}, X_{45}, X_{34}, X_{23} andX_{12}. This is sufficient to show that $\phi(X_{ij}) = X_{ij}$ whenever $i < j \leq 6$ and that $\phi(D_{ijk7}AD_{ijk7}) = D_{ijk7}AD_{ijk7}$ or $D_{ijk8}AD_{ijk8}$.

Now consider those $X \in \mathcal{S}_6$ that are of type (b). In particular, consider

$$\phi(D_{4567}AD_{4567}) = Z$$

. If $Z = D_{4567}AD_{4567}$, then we are done. If $Z = D_{4568}AD_{4568}$, then replace ϕ by the mapping $X \mapsto X_{78}\phi(X)X_{78}$. It can be shown (see the last section) that

$$(D_{ijk7}AD_{ijk7}, D_{4567}AD_{4567}) \neq (D_{ijk8}AD_{ijk8}, D_{4567}AD_{4567}).$$

Thus, for all $X \in \mathcal{S}_6$, $\phi(X) = X$.

Let $X_{ijk} = X_{ij}X_{ik}$. Then X_{ijk} is the type (I) matrix as defined in §8.1 with the following principal submatrices.

$$X_{ijk}(i,j,k) = I_5, \qquad X_{ijk}[i,j,k] = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}.$$

In a manner similar to that of section 7.3, we consider those matrices $X \in \mathcal{S}_5$ such that $(X, X_{ij}) = 6$, $(X, X_{ik}) = 6$ and $(X, X_{jk}) = 6$ for $i < j < k$. Then $X = X_{ijk}$ or X_{ijk}^t. If $\phi(X_{123}) = X_{123}^t$, then replace ϕ by the mapping $X \mapsto \phi(X)^t$. Thus $\phi(X_{123}) = X_{123}$. Note that $(X_{ijk}, X_{123}) = 5$ if and only if $i + 1 = j < 3 < k \leq 6$. But if $(X_{ijk}, X_{123}) = 5$, then $(X_{ijk}, X_{123}^t) = 4$. So $\phi(X_{12k}) = X_{12k}$ for $k = 4, 5, 6$. Using these newly fixed matrices, continue in the same manner until $\phi(X_{ijk}) = X_{ijk}$ for all X_{ijk} such that $1 \le i < j < k \le 6$.

Note that for any $X \in \mathbf{E}_6$, if $Y \in \mathbf{E}_6$ and $(Y, X) = 6$, then $Y = XZ$ for some $Z \in \mathcal{S}_6$. Thus, for all $i < j < k \le 6$, if Y is such that $(Y, X_{ijk}) = 6$ and $(Y, X_{78}) = 6$, then $Y = X_{ijk}X_{78}$. Thus, $\phi(X_{ijk}X_{78}) = X_{ijk}X_{78}$ for all $i < j < k \le 6$. In particular, let $Y = X_{123}X_{78}$, and consider those X such that $(YX, I_8) = 6$ and $(YX, X_{78}) = 5$. They will be of the form $X = YDAD$ where $D = D_{ijk7}$ and $i < j < k \le 6$. For each such X, define

$$f(X) = [(X_{12}, X), ..., (X_{56}, X), (D_{1237}AD_{1237}, X), ..., (D_{4567}AD_{4567}, X)].$$

One can show that $f(X) \neq f(Z)$ whenever $X \neq Z$ where X and Z are both of the form $YDAD$ with $D \neq D_{1237}$, D_{1238}; see the last section.

These 18 matrices together with those $X \in \mathcal{S}_6$ and those matrices of the form X_{ijk} for $i < j < k \le 6$ all have the property that $\phi(X) = X$. It can be shown that there are 37 linearly independent matrices among this group; see the last section. Given this, and the fact that

$$\phi(0) = U^* \begin{pmatrix} I_2 & 0 \\ 0 & 0_6 \end{pmatrix} U,$$

we see that

$$\phi(X) - \phi(0)$$

is completely determined. In particular, $\phi(X) = X$ for all $X \in \mathcal{E}_6$. It follows that the original affine map ϕ on V_6 has the form

$$X \mapsto P^t X P \qquad \text{or} \qquad X \mapsto P^t X^t P$$

for some $P \in \mathcal{E}_6$. Note that if $P, X \in \mathcal{E}_6$, there exists $\hat{P}, \hat{X} \in \mathbf{E}_6$ such that

$$P^t X P = U^* \begin{pmatrix} 0_2 & 0 \\ 0 & \hat{P}^t \hat{X} \hat{P} \end{pmatrix} U + U^* \begin{pmatrix} I_2 & 0 \\ 0 & 0_6 \end{pmatrix} U.$$

Thus, there exists a $\hat{P} \in \mathbf{E}_6$ such that

$$\psi(\hat{X}) = \hat{P}^t \hat{X} \hat{P} \text{ for all } \hat{X} \in \mathbf{E}_6 \qquad \text{or} \qquad \psi(\hat{X}) = \hat{P}^t \hat{X}^t \hat{P} \text{ for all } \hat{X} \in \mathbf{E}_6.$$

Since $\mathbf{E}_6$ spans $M_6(\mathbf{R})$, ψ on $M_6(\mathbf{R})$ has the desired form. □

As in the case of $\mathbf{E}_7$, the above proof would also show a similar result if we replace the linear map ψ on $M_6(\mathbf{R})$ satisfying $\psi(\mathbf{E}_6) = \mathbf{E}_6$ with either an affine map $\phi : V_6 \to V_6$ or a linear map $\hat{\phi}$: span $\mathcal{E}_6 \to$ span $\mathcal{E}_6$ satisfying $\phi(\mathcal{E}_6) = \mathcal{E}_6$ and preserving inner product on V_6.

4.9 MATLAB Programs

MATLAB Program for $\mathbf{H}_3$

In the proof of the linear preserver of $\mathbf{H}_3$, we stated that 12 matrices

$$D_1, D_2, D_3, H, X_1, \ldots, X_8$$

span $M_3(\mathbf{R})$. We put these 12 matrices as row vectors of the matrix "R". The rank command will then show that there are 9 linearly independent vectors among these 12 matrices.

```
a=(1+sqrt(5))/4;b=(-1+sqrt(5))/4;c=1/2; R=[-1 0 0 0 1 0 0 0 1; 1 0
0 0 -1 0 0 0 1;
  1 0 0 0 1 0  0 0 -1; a b c  b c -a  c -a -b;
 -a -b -c   b  c -a   c -a -b; -a b  c   -b  c -a   -c -a -b;
 -a -b  c   b  c  a   -c  a -b; -a b -c   -b  c  a    c  a -b;
  a  b  c  -b -c  a    c -a -b;  a -b c    b -c -a    c  a -b;
  a  b -c  -b -c -a   -c  a -b;  a -b -c   b -c  a   -c -a -b];
rank(R)
```

MATLAB Program for H_4

In the proof of the linear preserver of H_4, we stated that 24 specific matrices could be shown to span $M_4(\mathbf{R})$. We put these twelve matrices in row vector form stared in "R". The rank command will then show that there are 16 linearly independent vectors among these 24 matrices.

```
a=(1+sqrt(5))/4;b=(-1+sqrt(5))/4;c=1/2;
D(:,:,1)=[-1 0 0 0; 0 1 0 0; 0 0 1 0; 0 0 0 1];
D(:,:,2)=[ 1 0 0 0; 0 -1 0 0; 0 0 1 0; 0 0 0 1];
D(:,:,3)=[ 1 0 0 0; 0 1 0 0; 0 0 -1 0; 0 0 0 1];
D(:,:,4)=[ 1 0 0 0; 0 1 0 0; 0 0 1 0; 0 0 0 -1];
B(:,:,1)=[1 0 0 0; 0 a b c; 0 b c -a; 0 c -a -b];
B(:,:,2)=[a b 0 c; b c 0 -a; 0 0 1 0; c -a 0 -b];
B(:,:,3)=[c 0 b -a; 0 1 0 0; b 0 a c; -a 0 c -b];
```

```
B(:,:,4)=D(:,:,3)*B(:,:,1); B(:,:,5)=D(:,:,2)*B(:,:,2);
B(:,:,6)=D(:,:,1)*B(:,:,3); k=0; for i=1:4
  for j=1:6
    k=k+1; y=D(:,:,i)*B(:,:,j)*D(:,:,i);
    R(k,:)=[y(1,:) y(2,:) y(3,:) y(4,:)];
  end
end rank(R)
```

MATLAB Program for $\mathbf{F}_4$

In the proof of the linear preserver of $\mathbf{F}_4$, we stated that we could show that the 16 matrices of the form DA_iD for $i = 1, 2$ and $D = \text{diag}\,(1, \pm 1, \pm 1, \pm 1)$ were mapped to themselves by comparing the inner products of these matrices with those already fixed by ϕ. Below follows the MATLAB code comparing the inner products of these 16 matrices with those of C_i for $i = 1, 3, 5$ and 6. A simple comparison of the inner products will verify that these matrices must indeed be mapped to themselves. We put the 16 matrices in row vector form, storing them in 'y'. The other matrices are also on row vector form, stored in 'x'. Finally, we use the 'rank' command to show that there are 16 linearly independent matrices among the 26 listed.

```
e1=[1 0 0 0];e2=[0 1 0 0];e3=[0 0 1 0];e4=[0 0 0 1];
D=[1 1 1 1; 1 -1 1 1; 1 1 -1 1; 1 -1 -1 1;
   1 1 1 -1; 1 1 -1 -1; 1 -1 1 -1; 1 -1 -1 -1];
A(:,:,1)=eye(4)-ones(4)/2;
```

```
A(:,:,2)=[1 1 -1 -1;1 1 1 1;1 -1 1 -1;1 -1 -1 1]/2; k=0;
for j=1:8
  for i=1:2
    k=k+1;B=diag(D(j,:))*A(:,:,i)*diag(D(j,:));
    y(k,:)=[B(1,:) B(2,:) B(3,:) B(4,:)];
  end
end x=[-e1 e2 e3 e4; e1 -e2 e3 e4; e1 e2 -e3 e4; e1 e2 e3 -e4;
    e1 e2 e4 e3; e1  e2 -e4 e3; e2  e1  e3 e4;
   -e2 e1 e3 e4; e1  e3  e2 e4; e1 -e3  e2 e4];
y*[x(5,:);x(7,:);x(9:10,:)]'; rank([x;y])
```

MATLAB Program for $\mathbf{E}_8$

In the proof of the linear preserver of $\mathbf{E}_8$, we showed that $\phi(X) = X$ for

$$X = I_8, Q_1 = D_{18}AD_{18} \text{ and } X_{i(i+1)} \text{ for } i = 1, ..., 7.$$

We stated that by comparing the inner product of these matrices with the rest of the elements in $\mathcal{S}_6$, that we could show that $\phi(X) = X$ for all $X \in \mathcal{S}_6$. We store those X that are fixed in row vector form in "rset" and store matrices of the forms DAD, X_{ij} and Y_{ij} in row vector forms in "rA8", "rX8" and "rY8" respectively. Direct comparison of the inner product shows that each matrix must be fixed. We also stated that the matrices of the forms

$$I_8,\ DAD,\ X_{ij},\ Y_{ij},\ X_{ijk}, \text{ and } PDAD,$$

as defined in section 3.3, could be shown to span $M_8(\mathbf{R})$. We form these matrices and put them in row vector form stored in "rI", "rA8", "rX8", "rY8", "rP8" and 'rPA8" respectively. The rank command will then show that there are 64 linearly independent vectors among these matrices.

```
d2=[1 1 1 1 1 -1 -1 1;1 1 1 1 -1 1 -1 1;1 1 1 -1 1 1 -1 1;
    1 1 -1 1 1 1 -1 1;1 -1 1 1 1 1 -1 1;-1 1 1 1 1 1 -1 1;
    1 1 1 1 -1 -1 1 1;1 1 1 -1 1 -1 1 1;1 1 -1 1 1 -1 1 1;
    1 -1 1 1 1 -1 1 1;-1 1 1 1 1 -1 1 1;1 1 1 -1 -1 1 1 1;
    1 1 -1 1 -1 1 1 1;1 -1 1 1 -1 1 1 1;-1 1 1 1 -1 1 1 1;
    1 1 -1 -1 1 1 1 1;1 -1 1 -1 1 1 1 1;-1 1 1 -1 1 1 1 1;
    1 -1 -1 1 1 1 1 1;-1 1 -1 1 1 1 1 1;-1 -1 1 1 1 1 1 1];
d4=[1 1 1 -1 -1 -1 -1 1;-1 -1 -1 1 1 1 -1 1
    1 1 -1 1 -1 -1 -1 1;-1 -1 1 -1 1 1 -1 1
    1 -1 1 1 -1 -1 -1 1;-1 1 -1 -1 1 1 -1 1
    -1 1 1 1 -1 -1 -1 1;1 -1 -1 -1 1 1 -1 1
    1 1 -1 -1 1 -1 -1 1;-1 -1 1 1 -1 1 -1 1
    1 -1 1 -1 1 -1 -1 1;-1 1 -1 1 -1 1 -1 1
    -1 1 1 -1 1 -1 -1 1;1 -1 -1 1 -1 1 -1 1
    1 -1 -1 1 1 -1 -1 1;-1 1 1 -1 -1 1 -1 1
    -1 1 -1 1 1 -1 -1 1;1 -1 1 -1 -1 1 -1 1
    -1 -1 1 1 1 -1 -1 1;1 1 -1 -1 -1 1 -1 1
    1 1 -1 -1 -1 -1 1 1;1 -1 1 -1 -1 -1 1 1
```

```
    -1 1 1 -1 -1 -1 1 1;1 -1 -1 1 -1 -1 1 1
    -1 1 -1 1 -1 -1 1 1;-1 -1 1 1 -1 -1 1 1
    1 -1 -1 -1 1 -1 1 1;-1 1 -1 -1 1 -1 1 1
    -1 -1 1 -1 1 -1 1 1;-1 -1 -1 1 1 -1 1 1
    1 -1 -1 -1 -1 1 1 1;-1 1 -1 -1 -1 1 1 1
    -1 -1 1 -1 -1 1 1 1;-1 -1 -1 1 -1 1 1 1
    -1 -1 -1 -1 1 1 1 1];
d6=[1 -1 -1 -1 -1 -1 -1 1;-1 1 -1 -1 -1 -1 -1 1;
    -1 -1 1 -1 -1 -1 -1 1;-1 -1 -1 1 -1 -1 -1 1;
    -1 -1 -1 -1 1 -1 -1 1;-1 -1 -1 -1 -1 1 -1 1;
    -1 -1 -1 -1 -1 -1 1 1];
d_8=[d6;d4;d2;ones(1,8)];w=[1 1 1 1 1 1 1 -1]'; A=eye(8) - w*w'/4;
for i=1:64;
 a=diag(d_8(i,:))*A*diag(d_8(i,:)); A_8(:,:,i)=a;
 rA8(i,:)=[a(1,:) a(2,:) a(3,:) a(4,:) a(5,:) a(6,:) a(7,:) a(8,:)];
end
k=0;
for j=2:8
 for i=1:(j-1);
  a=eye(8); a(i,i)=0; a(j,j)=0;
  b=zeros(8); b(i,j)=1; b(j,i)=1;
  X=a+b; Y=a-b; k=k+1;
```

```
  rX8(k,:)=[X(1,:) X(2,:) X(3,:) X(4,:) X(5,:) X(6,:) X(7,:) X(8,:)];
  rY8(k,:)=[Y(1,:) Y(2,:) Y(3,:) Y(4,:) Y(5,:) Y(6,:) Y(7,:) Y(8,:)];
 end
end
k=0;
for m=3:8;
 for j=2:(m-1)
  for i=1:(j-1)
   k=k+1; P=eye(8); P(i,i)=0; P(j,j)=0;
   P(m,m)=0; P(i,j)=1; P(j,m)=1; P(m,i)=1;
   rP8(k,:)=[P(1,:) P(2,:) P(3,:) P(4,:) P(5,:) P(6,:) P(7,:) P(8,:)];
   P_8(:,:,k)=P;
  end
 end
end p=[zeros(1,7) 1; eye(7) zeros(7,1)]; for i=1:64
 P=p*A_8(:,:,i);
 rPA8(i,:)=[P(1,:) P(2,:) P(3,:) P(4,:) P(5,:) P(6,:) P(7,:) P(8,:)];
end
a=[1 zeros(1,8)]; rI=[a a a a a a a 1];
rset=[rI;rA8(1,:);rX8(1,:);rX8(3,:);rX8(6,:);rX8(10,:);
      rX8(15,:);rX8(21,:);rX8(28,:)];
ip=[rA8;rX8;rY8]*rset' rank([rI;rA8;rX8;rY8;rP8;rPA8])
```

MATLAB Program for $\mathbf{E}_7$

In the proof of the linear preserver of $\mathbf{E}_7$, we stated that we could show that the matrices of the form DAD and X_{ij}, both in S_6 were mapped to themselves by comparing the inner products of these matrices with those already fixed by ϕ. Below follows the MATLAB code comparing the inner products of these 63 matrices with those of $X_{i(i+1}$ for $i = 1, 2, 4, 5, 6, 7$. A simple comparison of the inner products verifies that these matrices must indeed be mapped to themselves. Since the matrix realizations used for $\mathbf{E}_7$ form a subset of those used for $\mathbf{E}_8$, we use the matrices previously defined in for $\mathbf{E}_8$. We put the 63 matrices in row vector form, storing them in "rA7" and "rX8" respectively. The other matrices are also on row vector form, stored in "rset". We also stated that these matrices together with I_8 and matrices of the form X_{ijk} as defined in section 3.3, could be shown to span the 50 dimensional subspace of $M_8(\mathbf{R})$. We store these new matrices in row vector form in "rI" and "rP7"respectively. The rank command will then show that there are 50 linearly independent vectors among these matrices.

```
rA7=rA8(8:42,:); rX7=[rX8(1:21,:);rY8(22:28)]; rP7=rP8(1:35,:);
P_7=P_8(:,:,36:56); for i=36:56
  P=diag([1,1,1,1,1,1,1,-1])*P_8(:,:,i)*diag([1,1,1,1,1,1,1,-1]);
  rP7(i,:)=[P(1,:) P(2,:) P(3,:) P(4,:) P(5,:) P(6,:) P(7,:) P(8,:)];
end
rset=[rI;rX7(1,:);rX7(3,:);rX7(10,:);rX7(15,:);rX7(21,:);rX7(28,:)];
ip=[rA7;rX7]*rset' rank([rI;rA7;rX7;rP7])
```

MATLAB Program for $\mathbf{E}_6$

In the proof of the linear preserver of $\mathbf{E}_6$, we stated that we could show that the matrices of the form X_{ij} were mapped to themselves and matrices of the form DAD were mapped to themselves or to $\hat{D}A\hat{A}$ (for D and $\hat{D}$ of particular forms) by comparing the inner products of these matrices with those already fixed by ϕ. Below follows the MATLAB code comparing the inner products of these matrices with those of $X_{i(i+1}$ for $i = 1, 2, 3, 4, 5, 7$. A simple comparison of the inner products will verify that these matrices must indeed be mapped to themselves. Since the matrix realizations used for $\mathbf{E}_7$ form a subset of those used for $\mathbf{E}_8$, we use the matrices previously defined in for $\mathbf{E}_8$. We put the matrices in row vector form, storing them in "rX6" and "rA6" respectively. The fixed matrices are also in row vector form, stored in "rset". Next, we fixed one of these matrices of the form DAD and compare inner products of the remaining with those fixed, whose row vectors are once again stored on "rset'. Comparison will once again verify that all matrices of the form DAD are mapped to themselves. We store the matrices of the form $PDAD$ (as defined in section 5.3) in row vector in "rZA6". Comparing inner products with those already fixed (whose row vector forms are once again stored in "rset"), shows that these matrices must be mapped to themselves. Finally, we stated that these matrices together with I_8 and matrices of the form X_{ijk} as defined in section 5.3, could be shown to span the 37 dimensional subspace of $M_8(\mathbf{R})$. We store these new matrices in row vector form in "rI" and "rP6"respectively. The rank command will then show that there are 37 linearly independent vectors among these matrices.

```
A_6=A_8(:,:,8:27); rA6=rA8(8:27,:); rX6=rX8(1:15,:); Y=[eye(6)
zeros(6,2);zeros(2,6) eye(2)-ones(2)]; rY=rY8(28,:);
rP6=rP8(1:20,:);
rset=[rI;rX6(1,:);rX6(3,:);rX6(6,:);rX6(10,:);rX6(15,:);rY];
ip=[rA6;rX6]*rset' rset=[rI;rX6;rY;rA6(1,:)]; ip=[rA6]*rset'
z=P_6(:,:,1,2,3)*Y; for i=1:20
  Z=z*A_6(:,:,i);
  rZA6(i,:)=[Z(1,:) Z(2,:) Z(3,:) Z(4,:) Z(5,:) Z(6,:) Z(7,:) Z(8,:)];
end rset=[rI;rX6;rY;rA6]; ip=[rZA6]*rset'
rank([rI;rA6;rX6;rY;rP6;rZA6(3:20,:)])
```

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