FRAMES OF ORTHOGONAL PROJECTIONS

by

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Abstract

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The primary aim of this thesis is to find and compare appropriate notions of distances on frames which arise from different contexts. A frame $\mathcal{E}$ is a collection $\{E_1, \ldots, E_r\}$ of mutually orthogonal projections in M_n whose sum is the identity matrix I. A frame may be identified with the pinching operator $A \mapsto \sum_{i=1}^{r} E_i A E_i$ in $\mathcal{B}(M_n)$, or with the coset of a certain subgroup of U_n (i.e., as a point in a generalized flag manifold).

Angles, analogous to those between a pair of subspaces (equivalently, projections), are defined between a pair of frames to measure the distance between them: Θ is precisely the set of canonical angles between two pinchings (considered as projections in $\mathcal{B}(M_n)$), and Φ_0, Φ_+ are derived from the union of the canonical angles between the constituent projections of two frames. Norm inequalities in both directions are found between these sets of angles. By viewing a frame as a coset, and the arguments of the spectrum of a unitary representative for the coset as angles, some additional relations are derived. The question of when frames are antipodal with respect to a certain natural metric is also addressed; results are obtained for dimensions $n = 2, 3, 4$.

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For my mother and father

Contents

Chapter 1

Introduction

To any direct sum decomposition of $\mathbb{C}^n$ into orthogonal subspaces one can associate, via the correspondence between subspaces and projections, a collection of orthogonal projections which sum to the identity. The space of these resolutions of the identity, in the case where the projections are ordered in some predetermined fashion, has been studied extensively by both Kovarik and Sherif [15, 16, 17, 25, 26], and I shall essentially follow their notation in referring to these objects as frames. A particularly attractive feature of frames is that a frame can be viewed from a variety of other perspectives as well, ranging from a special subalgebra of the set of $n \times n$ matrices M_n [5], to a point in a complex flag manifold [28], to a quantum measurement; this last interpretation is one which particularly intrigues me, and served as the motivation for this work.

A natural question is how should one define the distance between a pair of frames? As might be expected from the plethora of different viewpoints, there is no single 'best' candidate for a metric; a number of different alternatives exist, each with their respective strengths and weaknesses. These can be roughly grouped into three categories, depending on whether we interpret a frame as an object based in $\mathbb{C}^n$, M_n, or $\mathcal{B}(M_n)$. The main thrust of this work will be to compare the different notions of distance between frames.

The first chapter deals with preliminaries such as notation and a more detailed elaboration of some various interpretations of frames. A short section on majorization collects results which will be used later on. The next two chapters introduce distances based on the viewpoints of frames as measurements and cosets. The idea of defining angles between two frames is introduced in the fourth chapter, and with distances and angles based in $\mathbb{C}^n$, M_n, and $\mathcal{B}(M_n)$ in place, a number of relations and inequalities comparing the different quantities are derived. Finally, the last chapter closes with a discussion of when frames are maximally far apart (in a certain sense), and how spread out they are.

1.1 Notation

Three vector spaces will be of particular interest in this thesis: the n-dimensional complex (real) vector space $\mathbb{C}^n$ ($\mathbb{R}^n$), the space of $n \times n$ complex matrices M_n, and $\mathcal{B}(M_n)$, the space of (bounded) linear maps on M_n. Throughout this thesis n will always refer to the dimension of $\mathbb{C}^n$. We will generally use lowercase italic, uppercase italic, and script letters to denote elements of $\mathbb{C}^n$, M_n, and $\mathcal{B}(M_n)$ respectively.

1.1.1 Notation on $\mathbb{C}^n$ and $\mathbb{R}^n$

Let e_i be the vector in $\mathbb{C}^n$ whose only nonzero coordinate consists of a one in the ith position. Let $e = \sum_{i=1}^n e_i = (1, 1, \ldots, 1)$ and for any $x \in \mathbb{C}^n$, define $\operatorname{Tr} x = e^t x$. The inner product of two vectors $x, y \in \mathbb{C}^n$ will be written $(x, y) = y^* x$.

If $x = (x_1, \ldots, x_n) \in \mathbb{R}^n$, $x^\downarrow = (x_1^\downarrow, \ldots, x_n^\downarrow)$ and $x^\uparrow = (x_1^\uparrow, \ldots, x_n^\uparrow)$ will denote the vectors obtained by rearranging the coordinates x_i of x in decreasing and increasing order, respectively. Thus $x_1^\downarrow \geq \cdots \geq x_n^\downarrow$ and $x_1^\uparrow \leq \cdots \leq x_n^\uparrow$.

Let $x, y \in \mathbb{R}^n$. We will write $x \leq y$ if $x_i \leq y_i$ for all i. Recall that x is weakly majorized by y (written $x \prec_w y$) if

$$\sum_{i=1}^k x_i^\downarrow \leq \sum_{i=1}^k y_i^\downarrow, \qquad 1 \leq k \leq n. \tag{1.1}$$

If in addition

$$\sum_{i=1}^n x_i^\downarrow = \sum_{i=1}^n y_i^\downarrow \tag{1.2}$$

holds, x is majorized by y (written $x \prec y$). We will say $x \prec y$ strictly if $x \prec y$ and x is not a permutation of y.

A vector $x \in \mathbb{R}^n$ is a probability vector if $x \geq 0$ and $\operatorname{Tr} x = 1$. Finally, if $f : \mathbb{R} \to \mathbb{R}$ and $x = (x_1, \ldots, x_n)$, we will write $f(x)$ for the vector $(f(x_1), \ldots, f(x_n))$.

1.1.2 Notation on M_n

Let J_n be the $n \times n$ matrix which has each entry equal to $\frac{1}{n}$. If U is a unitary matrix, let $os(U)$ denote the associated orthostochastic matrix whose (i, j)-entry is $|U_{ij}|^2$. If

$P \in M_n$ is positive (semidefinite), that is, $(Px, x) \geq 0$ for all $x \in \mathbb{C}^n$, we will write $P \geq 0$. If P is a projection, $P^{\perp}$ will denote the complementary projection $I - P$.

The set of permutation, hermitian, skew-hermitian, and unitary matrices in M_n will be denoted by S_n, M_n^h, iM_n^h, and U_n respectively. The set of $n \times n$ density matrices (i.e., the set of positive semidefinite matrices of trace 1) will be denoted by Δ_n. (We will also use the same symbol to denote the set of probability vectors in $\mathbb{R}^n$; the context should eliminate any confusion.)

Let $A \in M_n$. We write $s(A)$ for the vector listing the singular values of A in decreasing order (so $s_1(A) \geq \cdots \geq s_n(A)$). If $A, B \in M_n^h$ then $\lambda(A)$ will similarly denote the vector listing the eigenvalues of A listed in decreasing order, and we will write $A \prec_w B$ (respectively $A \prec B$) if $\lambda(A) \prec_w \lambda(B)$ (respectively $\lambda(A) \prec \lambda(B)$).

The Schatten p-norm of A will be denoted by $\|A\|_p$ and the Ky Fan k-norm of A by $\|A\|_{(k)}$. In particular, we refer to the ∞-norm, 2-norm, and 1-norm as the bound norm, Frobenius norm, and trace norm, respectively. We use the same notation for the corresponding norms on $\mathbb{C}^n$.

1.1.3 Notation on $\mathcal{B}(M_n)$

The set of $n \times n$ (complex) matrices M_n is also a Hilbert space (called the Hilbert-Schmidt space) when given the inner product $\langle A, B \rangle = \operatorname{Tr} B^* A$. Thus all the usual conventions for operators on a Hilbert space apply to $\mathcal{B}(M_n)$ as well.

The identity map in $\mathcal{B}(M_n)$ will be denoted by id. For each $U \in M_n$ we define a map $\phi_U \in \mathcal{B}(M_n)$ by $\phi_U(A) = UAU^*$ for any $A \in M_n$. If $\mathcal{P} \in \mathcal{B}(M_n)$ is a projection, $\mathcal{P}^{\perp}$ will denote the complementary projection $id - \mathcal{P}$.

Let $\phi \in \mathcal{B}(M_n)$. If ϕ is a positive operator on the Hilbert space M_n (i.e., $\langle \phi(A), A \rangle \geq 0$ for all $A \in M_n$) we will write $\phi \geq 0$. If ϕ preserves the positive elements of the C^*-algebra M_n (i.e., $\phi(A) \geq 0$ whenever $A \geq 0$), we will say ϕ is positivity-preserving.

1.2 Realizations of Frames

In this section we will define what a frame is, introduce some related terminology, and elaborate on the various descriptions of frames mentioned in the introduction.

Definition 1.2.1. A *frame* $\mathcal{E}$ on $\mathbb{C}^n$ is an unordered finite collection $\{E_1, \ldots E_r\}$ of projections $E_i \in M_n$ which satisfy:

1. $E_iE_j = \delta_{ij}E_i$,

2. $\sum_{i=1}^r E_i = I$.

If the ordering of these projections is important, we will speak of the *ordered* frame $E = (E_1, \dots, E_r)$. (Note that ordered frames will be distinguished by ordinary capital letters and round parentheses instead of script letters and curly braces.) If the number of projections in $\mathcal{E}$ is important we will call $\mathcal{E}$ an r-frame.

For even more precision, suppose the rank of E_i is n_i, where, purely for convenience, we will always assume wolog that $n_1 \geq \cdots \geq n_r$. In this case we shall say $\mathcal{E}$ is a frame of type $(n_1, \dots, n_r)$. Two frames are said to be *isomorphic* if they are of the same type. The special frames of type $(1, \dots, 1)$ will be called *minimal* frames.

The manifold of ordered frames was examined by Kovarik [15] in the more general setting of idempotents on a Banach space instead of projections on a Hilbert space; together with Sherif, they compared the geodesics on this manifold to another naturally arising path [17]. We will speak more of this in chapter 3.

As already alluded to, frames can also be perceived in a number of other ways. In addition to the natural geometric interpretation of r-frames as direct sum decompositions of $\mathbb{C}^n$ into r orthogonal subspaces, we can view frames as objects more or less living in M_n or $\mathcal{B}(M_n)$, instead of in $\mathbb{C}^n$.

1.2.1 Frames as Pinchings

Let $\mathcal{E} = \{E_1, \dots, E_r\}$ be a frame. We can identify $\mathcal{E}$ with an operator in $\mathcal{B}(M_n)$ (which will be denoted by the same symbol $\mathcal{E}$) by defining

$$\mathcal{E}A = \sum_{i=1}^{r} E_iAE_i$$

for all $A \in M_n$. Following the notation of Davis [5], we shall call the map $\mathcal{E}$ a *pinching*. (This terminology arises because if we write A in block matrix form with respect to the direct sum decomposition $\mathbb{C}^n = \oplus_{i=1}^r \operatorname{Ran} E_i$ then $\mathcal{E}A$ is just the block diagonal of A). Davis has shown that pinchings are precisely those projections on M_n whose range is a (self-adjoint) subalgebra containing its commutant; thus pinchings, and hence frames, are characterized by these special subalgebras of M_n. We therefore identify a frame $\mathcal{E}$ with its associated pinching and also with the subalgebra that is the range of this pinching, and use the same symbol $\mathcal{E}$ for all three objects—the context will indicate the appropriate interpretation.

This illuminates some of the terminology in Definition 1.2.1; two frames are isomorphic if and only if their associated subalgebras are, and a frame is minimal if and only if its associated subalgebra has minimal dimension. A few other concepts will prove useful.

Definition 1.2.2. A frame $\mathcal{E}$ *refines* another frame $\mathcal{F}$ if the associated subalgebras satisfy $\mathcal{E} \subset \mathcal{F}$.

Definition 1.2.3. If $A \in M_n$ is normal, frame(A) is the frame associated to the subalgebra A', where A' is the commutant of A. (Thus frame(A) consists of the minimal projections of A'.) If frame(A) $= \mathcal{E}$ we will say that A is *adapted* to $\mathcal{E}$. Note that this is a special case of $\mathcal{E}A = A$, which is itself a (weaker) notion that A is particularly well-suited to $\mathcal{E}$.

1.2.2 Frames as Quantum Measurements

A vast number of papers have been written in the physics literature about the question of just what exactly happens during the measurement process in quantum mechanics, and how a measurement should be interpreted. Despite the long history of the problem, there is certainly no clear consensus and much remains unresolved. However, if one is not so much interested in the details of the measurement but only in the physical state of the system before and after the measurement (as will be in our case in avoiding the philosophical questions of what constitutes a quantum measurement), experimental evidence tells us unambiguously what happens to the system. It turns out that the effect of a measurement on a system is the same as that of a pinching, and it is thus that we will identify a frame with a measurement.

We give a brief review of the measurement process based on the well-known Copenhagen interpretation and von Neumann's idea of a reduction of the state [20]; however, we are mainly interested in what happens to the state of the system (since that is how a pinching relates to a measurement) and not so much how or why.

In quantum mechanics, the state of a physical system is represented by a unit vector v in some Hilbert space $\mathcal{H}$, which, as our results are primarily of a finite-dimensional nature, we will take to be $\mathbb{C}^n$ for simplicity. Since the phase of v is not physically observable (i.e., both v and $e^{i\theta}v$ represent the same physical state), it is convenient to work instead with the density matrix vv^* which contains the same information, but without the phase arbitrariness.

More generally, one could prepare a statistical ensemble of states $v_i v_i^*$ with the ith state forming a fraction p_i of the whole. For obvious reasons, the density matrix

$\sum_i p_i v_i v_i^*$ is called a *mixed* state, in contrast to the rank one projections vv^* which are called *pure* states.

Physical observables, such as the spin of a particle, are represented by self-adjoint operators on $\mathcal{H}$. The possible values which can be measured for such an observable are given precisely by its spectrum. By the spectral theorem, we can write a physical observable H as $\sum_{i=1}^n \lambda_i P_i$, where the eigenvalues λ_i of H are distinct, and for simplicity we suppose first that each projection P_i is rank one.

Then if one measures H for a pure state A, one obtains the result λ_i with probability equal to $\operatorname{Tr} P_i A$. After the measurement, the system is found to be in the state P_i. If we consider performing a measurement on a large ensemble of identical states A, a fraction $\operatorname{Tr} P_i A$ will be found in the state P_i after the measurement, so as a whole, we obtain an ensemble given by the density matrix

$$\sum_i (\operatorname{Tr} P_i A) P_i = \sum_i P_i A P_i,$$

which is just the pinching of A by the minimal frame of projections $\{P_1, \ldots, P_n\}$. The foregoing clearly also applies to general ensembles represented by mixed states and holds even when the projections P_i are not necessarily rank one.

Thus we can identify a pinching $A \mapsto \sum_{i=1}^r E_i A E_i$ with respect to a frame $\mathcal{E} = \{E_1, \ldots, E_r\}$ with a quantum measurement of an observable whose spectral projections are given by $\mathcal{E}$. Note that the measured values of the observable (i.e., the eigenvalues) play no role in determining the ensemble output by a measurement, so we may speak of a measurement with respect to the frame $\mathcal{E}$. (In the case where the frame $\mathcal{E}$ is minimal, we shall say that the measurement is *complete.*) For the most part, we shall henceforth identify pinchings with quantum measurements.

1.2.3 Frames as Cosets

An ordered frame $E = (E_1, \ldots, E_r)$ of type $(n_1, \ldots, n_r)$ can be viewed as a sequence of nested subspaces $0 \subset M_1 \subset \cdots \subset M_r = \mathbb{C}^n$, where M_k is the range of $\sum_{i=1}^k E_i$; from this vantage point, the space of all ordered frames of a fixed type $(n_1, \ldots, n_r)$ is a complex flag manifold. These manifolds are homogeneous spaces which have been studied quite extensively in the literature; the presence of a natural Riemannian metric on these manifolds provides an obvious candidate for a distance function on ordered frames.

To obtain the space of all unordered frames of a fixed type, it is in general necessary to mod out the action of the symmetric group. We show how to identify cosets in the resulting coset space with frames.

Let M be the space of all frames of a fixed type $(n_1, \ldots, n_r)$, where as usual, we assume $n_1 \geq \ldots \geq n_r$. Fix a frame $\mathcal{E} = \{E_1, \ldots, E_r\}$ in M. We will view $\mathcal{E}$ as the subalgebra of all block diagonal matrices in M_n, and write $\mathcal{E} = M_{n_1} \oplus \cdots \oplus M_{n_r}$. Thus M can be viewed as the space of subalgebras isomorphic to $\mathcal{E}$.

Then for $U \in U_n$, $\mathcal{A} \in M$, the map

$$(U, \mathcal{A}) \to \phi_U(\mathcal{A}) = \{\phi_U(A) = UAU^* : A \in \mathcal{A}\}$$

is a transitive group action of the Lie group U_n on M. The isotropy group fixing $\mathcal{E}$ is readily seen to be the Lie subgroup H generated by block diagonal unitaries and block permutations, that is,

$$\begin{aligned} H &= \{U \text{unitary} : UE_jU^* = E_{\sigma(j)} \text{ for some permutation } \sigma \text{ on } r \text{ elements}\} \\ &= \{(U_1 \oplus \cdots \oplus U_r)\rho : U_j \in M_{n_j} \text{ is unitary}, \rho \text{ is a block permutation}\}. \end{aligned}$$

By a block permutation we mean a block matrix which has precisely one non-zero block (which will be an identity matrix) in each block row and column. Note that a block permutation only permutes blocks of the same size. Equivalently, H is the normalizer of the subgroup of block diagonal unitaries. In any case, M can be identified with the coset space U_n/H, as follows.

Given a frame $\mathcal{F} = \{F_1, \ldots, F_r\}$ in M, where $\operatorname{rank} F_i = n_i$, let U be a unitary such that $F_i = UE_iU^*$. We can then identify $\mathcal{F}$ with the coset of H in U_n represented by U. In particular, our fixed frame $\mathcal{E}$ can be represented by the identity matrix I. Conversely, given a representative U of a coset in U_n/H, we identify the coset containing U with the frame consisting of the projections $F_i = UE_iU^*$.

To sum up, a frame $\mathcal{F}$ in M can be represented as:

1. a collection of orthogonal projections $\{F_1, \ldots, F_r\}$ summing to the identity,
2. the pinching (or quantum measurement) $\mathcal{F}A = \sum_{i=1}^{r} F_iAF_i$,
3. the subalgebra of matrices in the range of the pinching $\mathcal{F}$,
4. the coset of a unitary U which satisfies $F_iU = UE_{\sigma(i)}$ for some permutation σ.

1.3 Some results concerning majorization

We collect here some theorems about majorization which will prove useful later on. A classic and exhaustive reference for majorization is [18], although the subject dates much further back to Hardy, Littlewood, and Polya [10]. A more recent introduction is Ando's excellent survey article [2]. Many books on matrix analysis will also devote a chapter or more to the topic—see for example [4, 12]. For a treatment of majorization from a physicist's viewpoint, see [1] (note that they use the reverse notation $x \succ y$ to denote that x is majorized by y). A survey of more recent results is given in [3].

We begin by quoting a standard result relating majorization to doubly stochastic matrices. Note that this and all other results in this section may be found in [2].

Definition 1.3.1. A matrix $S \in M_n$ is *doubly stochastic* if

$$\begin{aligned} S_{ij} &\geq 0 \qquad \text{for all } i, j, \\ \sum_{i=1}^{n} S_{ij} &= 1 \qquad \text{for all } i, \\ \sum_{j=1}^{n} S_{ij} &= 1 \qquad \text{for all } j. \end{aligned}$$

These three conditions are equivalent, respectively, to the conditions that S is positivity-preserving ($Sx \geq 0$ whenever $x \geq 0$), trace-preserving ($\operatorname{Tr} Sx = \operatorname{Tr} x$ for all vectors x), and unital ($Se = e$). If there exists a unitary U such that $S_{ij} = |U_{ij}|^2$ for all i, j then S is called *orthostochastic*.

Theorem 1.3.2. *Let $x, y \in \mathbb{R}^n$. The following statements are equivalent:*

1. $x \prec y$.
2. *x lies in the convex hull of $\{\sigma y : \sigma \in S_n\}$.*
3. *$x = Sy$ for some doubly stochastic matrix S.*

This theorem can be generalized.

Definition 1.3.3. A linear map $\phi : M_n \to M_n$ is *doubly stochastic* if it is positivity-preserving (i.e., $\phi(A) \geq A$ whenever $A \geq 0$), unital (i.e., $\phi(I) = I$), and trace-preserving (i.e., $\operatorname{Tr} \phi(A) = \operatorname{Tr} A$ for all $A \in M_n$).

Theorem 1.3.4. *Let $A, B \in M_n^h$. The following statements are equivalent:*

1. $A \prec B$.

2. *There exist unitary matrices U_j and positive numbers $t_j > 0$ such that*

$$\sum_{j=1}^{N} t_j = 1 \text{ and } A = \sum_{j=1}^{N} t_j U_j B U_j^*.$$

3. $A = \phi(B)$ *for a doubly stochastic map* ϕ.

Remark 1.3.5. The preceding theorem is particularly useful for us because all pinchings are doubly stochastic maps, so $\mathcal{E}A \prec A$ for any pinching $\mathcal{E}$ and any hermitian A.

Majorization relations are particularly useful due to their intimate relation to norm inequalities.

Definition 1.3.6. A permutation-invariant norm Ψ on $\mathbb{C}^n$ which also satisfies $\Psi(x) = \Psi(|x|)$ for all $x \in \mathbb{C}^n$ is called a *symmetric gauge function.* A norm $\|\cdot\|$ on M_n which satisfies $\|UAV\| = \|A\|$ for any unitaries U, V is called a *unitarily invariant norm.* A unitarily invariant norm $\|\cdot\|$ is called a *Q-norm* if there exists a unitarily invariant norm $|||\cdot|||$ for which $\|A\|^2 = |||A^*A|||$ holds for all $A \in M_n$.

Theorem 1.3.7.

1. *Let $x, y \in \mathbb{C}^n$. Then $\Psi(x) \leq \Psi(y)$ for every symmetric gauge function Ψ iff $|x| \prec_w |y|$.*

2. *Let $A, B \in M_n$. Then $\|A\| \leq \|B\|$ for every unitarily invariant norm $\|\cdot\|$ iff $s(A) \prec_w s(B)$.*

Convex functions are also useful in that they essentially preserve the majorization relation.

Theorem 1.3.8. *Let $x, y \in \mathbb{R}^n$ and let $f : \mathbb{R} \to \mathbb{R}$ be a convex function. Then we have*

1. $x \prec y \Rightarrow f(x) \prec_w f(y)$.

2. *If in addition f is increasing,* $x \prec_w y \Rightarrow f(x) \prec_w f(y)$.

Finally, we state a proposition which shows that majorization is preserved when vectors are combined.

Proposition 1.3.9. *If*

$$x = (x_1, \dots, x_p) \prec y = (y_1, \dots, y_p)$$

and

$$u = (u_1, \dots, u_q) \prec v = (v_1, \dots, v_q)$$

then

$$(x, u) = (x_1, \dots, x_p, u_1, \dots, u_q) \prec (y, v) = (y_1, \dots, y_p, v_1, \dots, v_q)$$

The result also holds if all majorizations $\prec$ *are changed to weak majorizations* $\prec_w$.

Chapter 2

Distance based on Majorization

When one performs a measurement $\mathcal{E}$ on a pure state A, the resulting state $\mathcal{E}A$ need not be pure; indeed, $\mathcal{E}A$ will usually be a mixed state. In general, measuring any state A with respect to a frame $\mathcal{E}$ results in a more mixed up state, in the sense that $\mathcal{E}A$ is majorized by A (see remark 1.3.5). For example, consider the simple case of $\mathcal{E} = \{e_1e_1^*, e_2e_2^*\}$ and $A = vv^*$ where $v = \cos\theta e_1 + \sin\theta e_2$. In this case,

$$\mathcal{E}A = \begin{pmatrix} \cos^2\theta & 0 \\ 0 & \sin^2\theta \end{pmatrix}$$

is a mixed state for any $\theta \in (0, \frac{\pi}{2})$. Note that as θ increases from 0 to $\frac{\pi}{4}$, the orthonormal basis containing v moves farther and farther from the standard basis $\{e_1, e_2\}$ while $\mathcal{E}A$ becomes more and more 'mixed up', in the sense of majorization; at $\theta = \frac{\pi}{4}$, frame(A) is as far as possible from $\mathcal{E}$ while $\mathcal{E}A = \frac{1}{2}I$ is as mixed up as possible.

We would like to utilize this correlation to define a distance between two frames $\mathcal{E}$ and $\mathcal{F}$. Suppose A is a state unaffected by measurement with respect to $\mathcal{E}$, so $\mathcal{E}A = A$. If $\mathcal{F}$ is close to $\mathcal{E}$ one would expect that measuring A wrt $\mathcal{F}$ does not mess A up too much. The farther $\mathcal{F}$ is from $\mathcal{E}$, the more mixed up one would expect $\mathcal{F}A$ to be. In order to use this idea to quantify how far apart $\mathcal{E}$ and $\mathcal{F}$ are, we need a way to measure how badly a state is mixed up.

A natural measure of the degree of disorder inherent in a state A is the (von Neumann) entropy $-\operatorname{Tr} A \ln A$ of the state. Entropy has long been used to reflect the uncertainty or randomness of a system (think of the eigenvalues of a state A as probabilities) in many contexts; von Neumann's approach [20] was motivated by quantum mechanics. Shannon [24] viewed entropy from an information theoretic viewpoint; for him, the uncertainty in the state measures the amount of information carried by the state. A nice reference on entropy as it relates to quantum mechanics is [21].

Since the entropy function $f(t) = -t\ln t$ is concave and $\mathcal{E}A \prec A$, it follows by Theorem 1.3.8 that $\operatorname{Tr} f(\mathcal{E}A) \geq \operatorname{Tr} f(A)$, that is, the entropy increases after performing a measurement, as one would expect. It would be ideal if such a natural measure of disorder yielded a distance on the space of frames. Could the maximum increase in entropy,

$$\sup\{\operatorname{Tr}(f(\mathcal{F}A) - f(A)) : \mathcal{E}A = A, A \in \Delta_n\} = \sup_{A\in\Delta_n} \operatorname{Tr}(f(\mathcal{F}\mathcal{E}A) - f(\mathcal{E}A)), \quad (2.1)$$

give a distance between $\mathcal{E}$ and $\mathcal{F}$?

To answer this question, it will be useful to introduce the following lemma.

Lemma 2.0.10. *Let $\mathcal{E}$ be the minimal frame $\{E_1, E_2, \ldots, E_n\}$ where $E_i = e_i e_i^*$. Let $\mathcal{F} = \{F_1, \ldots, F_n\}$ and $\mathcal{G} = \{G_1, \ldots, G_n\}$ where $F_i = UE_iU^*$ and $G_i = VE_iV^*$ for some unitaries U, V. Let $A = \sum_{i=1}^n \lambda_i G_i$, so $\mathcal{G}A = A$. Then the spectrum of $\mathcal{F}A$ is given by $S\lambda$ where $S = os(U^*V)$ is the orthostochastic matrix with entries $S_{ij} = |(U^*V)_{ij}|^2$ and $\lambda = (\lambda_1, \ldots, \lambda_n)$.*

Proof. We have

$$\begin{aligned}
\mathcal{F}A &= \sum_{j=1}^n UE_jU^*(\sum_{i=1}^n \lambda_i VE_iV^*)UE_jU^* \\
&= \sum_{i,j} \lambda_i Ue_je_j^*U^*Ve_ie_i^*V^*Ue_je_j^*U^* \\
&= \sum_{i,j} \lambda_i |(V^*U)_{ij}|^2 (Ue_j)(Ue_j)^*.
\end{aligned}$$

This says that the spectrum of $\mathcal{F}A$ is $\{\sum_{i=1}^n |(V^*U)_{ij}|^2\lambda_i : j = 1, \ldots, n\}$ as claimed. □

For the special case $\mathcal{G} = \mathcal{E}$ in the lemma, the spectrum of $\mathcal{F}A$ is given by $os(U^*)\lambda$. Thus if $\mathcal{E}$ and $\mathcal{F}$ are minimal frames as in the lemma,

$$\sup_{A\in\Delta_n} \operatorname{Tr}(f(\mathcal{F}\mathcal{E}A) - f(\mathcal{E}A)) = \sup_{p\in\Delta_n} \operatorname{Tr}(f(os(U^*)p) - f(p)).$$

The following proposition shows that in this case, the supremum is given by the maximal entropy of the row vectors of $os(U)$, namely

$$\max_{i=1}^{n} \sum_{j=1}^n f(|U_{ij}|^2).$$

Proposition 2.0.11. *Let S be a doubly stochastic matrix and $f(x) = -x \ln x$. Define $H : \mathbb{R}_+^n \to \mathbb{R}_+$ by $H(p) = \mathrm{Tr}(f(Sp) - f(p))$. Then H attains its maximum on Δ_n at some extreme point e_i.*

Proof. Suppose $p \in \Delta_n$ is not an extreme point. Then there are two indices j, k for which $p_j, p_k \neq 0$; wolog assume $j = 1, k = 2$, and $p_j \geq p_k$. Let $q = e_1 - e_2$. Note that for each $x \in [-p_1, p_2]$ the vector $p(x) = p + xq$ lies in Δ_n, and that both $p - p_1 q$, $p + p_2 q$ have (at least) one more zero coordinate than p. I will show that the function $g(x) = H(p(x))$ attains its maximum on $[-p_1, p_2]$ at an endpoint; hence $H(r) \geq H(p)$ for some $r \in \Delta_n$ with more zero coordinates than p, and the proposition follows.

It thus suffices to prove that g is convex. Let I denote the set of indices i for which $(Sp)_i > 0$. Note that if $x \in (-p_1, p_2)$, then $(Sp(x))_i > 0$ as well. Let I' be the set of indices $i \in I$ for which not both S_{i1}, S_{i2} are zero. Then

$$g(x) = \mathrm{Tr}(f(Sp(x)) - f(p(x))) = \sum_{i \in I} f((Sp(x))_i) - \sum_{i=1}^{n} f(p_i + xq_i).$$

Differentiating twice gives

$$\begin{aligned}
g''(x) &= \sum_{i \in I} f''((Sp(x))_i)(S_{i1} - S_{i2})^2 - f''(p_1 + x) - f''(p_2 - x) \\
&= \sum_{i \in I} -\frac{(S_{i1} - S_{i2})^2}{\sum_{j=1}^n S_{ij} p(x)_j} + \frac{1}{p_1 + x} + \frac{1}{p_2 - x} \\
&\geq \frac{1}{p_1 + x} + \frac{1}{p_2 - x} - \sum_{i \in I'} \frac{S_{i1}^2 + S_{i2}^2}{\sum_{j=1}^n S_{ij} p(x)_j} \\
&\geq \frac{1}{p_1 + x} + \frac{1}{p_2 - x} - \sum_{i \in I'} \frac{S_{i1}^2 + S_{i2}^2}{S_{i1} p(x)_1 + S_{i2} p(x)_2} \\
&\geq \frac{1}{p_1 + x} + \frac{1}{p_2 - x} - \sum_{i \in I'} \left(\frac{S_{i1}^2}{S_{i1}(p_1 + x)} + \frac{S_{i2}^2}{S_{i2}(p_2 - x)}\right) \\
&\geq \frac{1}{p_1 + x} + \frac{1}{p_2 - x} - \frac{1}{p_1 + x} - \frac{1}{p_2 - x} = 0
\end{aligned}$$

where the last inequality holds because $\sum_{i \in I'} S_{ij} \leq 1$. Thus g is convex as desired. □

As an aside, note that only the concavity of the entropy function f is required to show that $\mathrm{Tr} f(\mathcal{E}A) \geq \mathrm{Tr} f(A)$, so one might use some other concave function instead of entropy to measure how much more mixed a state is after a measurement.

In fact, if g is an operator concave function, the much stronger operator inequality $g(\mathcal{E}A) \geq \mathcal{E}g(A)$ (see [4, Theorem V.2.1]) holds, so one might wonder if the preceding proposition holds for any operator concave function instead of just for the entropy function. That this is not the case may be seen by the following example.

Example 2.0.12. Let $g(x) = \frac{x-\lambda x^2}{x+\lambda}$, $p = (\frac{1}{2}, 0, \frac{1}{2}, 0)$, and

$$S = \frac{1}{2}\begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix}.$$

If $\lambda \in (0, \frac{1}{2})$ then

$$\operatorname{Tr}(g(Sp) - g(p)) > \operatorname{Tr}(g(Se_i) - g(e_i))$$

for any index i. Thus the function $\operatorname{Tr}(g(Sp) - g(p))$ on Δ_n need not be maximized at an extreme point, even though g is operator concave.

Proposition 2.0.11 shows that if $\mathcal{E}$ and $\mathcal{F}$ are minimal frames, the quantity in (2.1) is just $\max_i \operatorname{Tr} f(\mathcal{F}E_i)$ and so is very easy to compute. However, it is not in general symmetric in $\mathcal{E}$ and $\mathcal{F}$; consider $\mathcal{E}$ and $\mathcal{F}$ as in Lemma 2.0.10 with

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

and $V = I$. Moreover, even the symmetrized version $\max_i(\operatorname{Tr}(\mathcal{F}E_i), \operatorname{Tr}(\mathcal{E}F_i))$ fails to satisfy the triangle inequality; it suffices to consider the simple case $n = 2$ and any three frames reasonably close together.

One might consider using an average instead to obtain a distance on minimal frames:

$$\sum_{i=1}^{n} \operatorname{Tr} f(\mathcal{F}E_i), \text{ or } \int_{\Delta_n} \operatorname{Tr} f(\mathcal{F}\mathcal{E}A) - \operatorname{Tr} f(\mathcal{E}A) dA.$$

These candidates have the advantage of distinguishing between frames much better than (2.1) but also fail to satisfy the triangle inequality.

We can tweak the first candidate to

$$d(\mathcal{E}, \mathcal{F}) = (\sum_{i=1}^{n} \operatorname{Tr} f(\mathcal{F}E_i))^p$$

so that it satisfies the triangle inequality locally for $p \leq \frac{1}{2}$.

However this tweaked version is not particularly nice; if $\mathcal{E}(t)$ is a smooth path through $\mathcal{E}(0) = \mathcal{E}$ and $\delta(t) = d(\mathcal{E}, \mathcal{E}(t)) + d(\mathcal{E}(t), \mathcal{G}) - d(\mathcal{E}, \mathcal{G})$, then $\delta'(0)$ is infinite. The entropy function, though a natural measure of the disorder of a state, is problematic as a progenitor for a distance on frames; its behaviour at the origin seems to preclude any possibility of using it to obtain a reasonable metric for frames.

Faced with this difficulty, yet still wishing to use the increase in disorder of $\mathcal{F}\mathcal{E}A$ over $\mathcal{E}A$ as a distance, we consider replacing the entropy function $-t\ln t$ by some other concave function $f(t)$. We would like $f(A) = 0$ for pure states A; this imposes the condition $f(0) = f(1) = 0$. Probably the simplest such concave function is $f(x) = x - x^2$. In this case, if $\mathcal{E}, \mathcal{F}$ are minimal frames,

$$\begin{aligned}
\sum_{i=1}^{n} \operatorname{Tr} f(\mathcal{F}E_i) &= \sum_{i=1}^{n} \operatorname{Tr}(\mathcal{F}E_i - (\mathcal{F}E_i)^2) \\
&= \sum_{i=1}^{n} 1 - \langle \mathcal{F}E_i, \mathcal{F}E_i \rangle \\
&= \sum_{i=1}^{n} \langle E_i, E_i \rangle - \langle \mathcal{F}E_i, E_i \rangle \\
&= \sum_{i=1}^{n} \langle \mathcal{F}^{\perp}\mathcal{E}E_i, E_i \rangle \\
&= \|\mathcal{F}^{\perp}\mathcal{E}\|_2^2
\end{aligned}$$

since $E_1, \ldots, E_n$ can be extended to an orthonormal basis for M_n, and any matrix in such a basis which is not one of the matrices E_i lies in the kernel of $\mathcal{F}^{\perp}\mathcal{E}$.

But, viewing $\mathcal{E}$ and $\mathcal{F}$ as projections on M_n,

$$(\mathcal{E} - \mathcal{F})^2 = \mathcal{E}\mathcal{F}^{\perp} + \mathcal{F}\mathcal{E}^{\perp} = \begin{pmatrix} \mathcal{E}\mathcal{F}^{\perp}\mathcal{E} & 0 \\ 0 & \mathcal{E}^{\perp}\mathcal{F}\mathcal{E}^{\perp} \end{pmatrix} \tag{2.2}$$

when written in block matrix form with respect to the direct sum decomposition $M_n = \mathcal{E}M_n \oplus \mathcal{E}^{\perp}M_n$. Hence

$$\|\mathcal{E} - \mathcal{F}\|_2^2 = \|\mathcal{F}^{\perp}\mathcal{E}\|_2^2 + \|\mathcal{E}^{\perp}\mathcal{F}\|_2^2 = 2\|\mathcal{F}^{\perp}\mathcal{E}\|_2^2$$

since $\mathcal{E}^{\perp}\mathcal{F}$ and $\mathcal{F}^{\perp}\mathcal{E}$ have the same singular values if $\mathcal{E}$ and $\mathcal{F}$ are projections of the same rank (see [4, p.201]).

Thus using the concave function $x - x^2$ to measure how mixed a state is leads to a very natural distance for minimal frames:

$$\sqrt{2\sum_{i=1}^{n} \operatorname{Tr} f(\mathcal{F}E_i)} = \|\mathcal{E} - \mathcal{F}\|_2.$$

Two obvious questions are:

1. For general frames $\mathcal{E}$ and $\mathcal{F}$, will $\|\mathcal{E} - \mathcal{F}\|_2$ also reflect the idea that the more a measurement $\mathcal{F}$ messes up a state adapted to $\mathcal{E}$, the further $\mathcal{F}$ is from $\mathcal{E}$?

2. Do we retain the 'messing up' idea if we replace the 2-norm of $\mathcal{E} - \mathcal{F}$ by an arbitrary unitarily invariant norm?

The answer is yes to both questions, as we show in the following theorem.

Proposition 2.0.13. *Suppose $\mathcal{E}, \mathcal{F}, \mathcal{G}$ are isomorphic frames satisfying $\mathcal{G}\mathcal{E}A \prec \mathcal{F}\mathcal{E}A$ for all density matrices A. Then $\|\mathcal{G} - \mathcal{E}\| \geq \|\mathcal{F} - \mathcal{E}\|$ for all unitarily invariant norms.*

Proof. It is easy to see that if A, B are two hermitian matrices then

$$A \prec B \iff xA + yI \prec xB + yI \quad \forall x, y \in \mathbb{R}, x \neq 0.$$

Since any hermitian matrix B may be written $B = xA + yI$ for some density matrix A and real numbers x, y it follows that

$$\mathcal{G}\mathcal{E}B = x\mathcal{G}\mathcal{E}A + yI \prec x\mathcal{F}\mathcal{E}A + yI = \mathcal{F}\mathcal{E}B,$$

and so for all $B \in M_n^h$ we have

$$\begin{aligned}
&\mathcal{G}\mathcal{E}B \prec \mathcal{F}\mathcal{E}B \\
\Rightarrow&\|\mathcal{G}\mathcal{E}B\|_2 \leq \|\mathcal{F}\mathcal{E}B\|_2 && \text{by Theorems 1.3.7,1.3.8} \\
\Rightarrow&\langle \mathcal{E}\mathcal{G}\mathcal{E}B, B\rangle \leq \langle \mathcal{E}\mathcal{F}\mathcal{E}B, B\rangle \\
\Rightarrow&\langle \mathcal{E}(\mathcal{F} - \mathcal{G})\mathcal{E}B, B\rangle \geq 0.
\end{aligned}$$

Since $\mathcal{E}(\mathcal{F} - \mathcal{G})\mathcal{E}$ is self-adjoint and preserves M_n^h, it has an orthonormal basis of eigenvectors which are hermitian matrices. Thus the eigenvalues of $\mathcal{E}(\mathcal{F} - \mathcal{G})\mathcal{E}$ are all positive, so $\mathcal{E}(\mathcal{F} - \mathcal{G})\mathcal{E} \geq 0$. Thus

$$\begin{aligned}
&0 \leq \mathcal{E}\mathcal{G}\mathcal{E} \leq \mathcal{E}\mathcal{F}\mathcal{E} \leq \mathcal{E} \\
\Rightarrow&\mathcal{E} \geq \mathcal{E}\mathcal{G}^{\perp}\mathcal{E} \geq \mathcal{E}\mathcal{F}^{\perp}\mathcal{E} \geq 0 \\
\Rightarrow&s(\mathcal{G}^{\perp}\mathcal{E}) \geq s(\mathcal{F}^{\perp}\mathcal{E}) \\
\Rightarrow&\|\mathcal{G} - \mathcal{E}\| \geq \|\mathcal{F} - \mathcal{E}\|, && \text{for all u.i. norms,}
\end{aligned}$$

where the last inequality follows from [4, Ex VII.1.11]. □

We conclude that $\|\mathcal{E} - \mathcal{F}\|$ is a good distance to measure how far apart two frames are, based on the idea of a subsequent measurement $\mathcal{F}$ messing up an earlier measurement $\mathcal{E}$. However, nice as this distance is, it is still not ideal; for instance, it does not arise from any Riemannian metric and need not have any geodesics. Moreover, it is quite removed from our intuition of frames as a collection of orthogonal subspaces in $\mathbb{C}^n$; it would be nice to have a distance which reflects this intuition. In the next two chapters we will address these issues by considering other distances.

Chapter 3

Geometry of Isomorphic Frames

In this section we identify the space of all frames of a fixed type with a coset space, which, as noted in section 1.2.3, is essentially a complex flag manifold. This allows us to apply some basic Lie theory, so we can follow the prescription of any of a number of texts [11, 14] to introduce a natural Riemannian metric and its associated distance on this space of isomorphic frames. We note that the geometry obtained in this manner coincides with that found by Kovarik [15], and describe the geodesics and how to compute the distance between two frames.

We begin by fixing some notation (which is mostly standard and generally follows [11]) and quoting some general results of Lie theory. Let G be a Lie group with identity e and let H be a closed Lie subgroup. Let $\mathfrak{g}$ and $\mathfrak{h}$ denote the Lie algebras of G and H respectively. If $x \in G$, let $L_x, R_x : G \to G$ denote the left and right translations by x respectively, that is, $L_x(y) = xy$, $R_x(y) = yx$ for all $y \in G$. Let π be the quotient map from G onto G/H and give G/H the quotient topology. If $g \in G$ we will write $\hat{g} = \pi(g) = gH$ for the (left) coset of H represented by g. For each $x \in G$, L_x induces a map $\hat{L}_x : G/H \to G/H$ defined by $\hat{L}_x(yH) = xyH$ (here $y \in G$).

Note that

$$\hat{L}_x \circ \pi = \pi \circ L_x \text{ for any } x \in G. \tag{3.1}$$

By [11, Theorem II.4.2] G/H has a unique analytic structure such that G is a Lie transformation group of G/H; that is, the map $(x, yH) \mapsto xyH$ $(x, y \in G)$ is an analytic map of $G \times G/H$ onto G/H. We will always endow G/H with this analytic structure. Note in particular that both π and $\hat{L}_x$ are analytic.

For each $x \in G$ we define an automorphism $\phi_x : G \to G$ by $\phi_x(g) = xgx^{-1}$. This induces a mapping $\mathrm{Ad} : G \to GL(\mathfrak{g})$, $\mathrm{Ad}(x) = d(\phi_x)_e$, the adjoint representation of G. The adjoint representation of $\mathfrak{g}$ will be denoted by the lowercase symbol ad; here ad : $\mathfrak{g} \to GL(\mathfrak{g})$ maps an element $X \in \mathfrak{g}$ into the function $\mathrm{ad}_X : \mathfrak{g} \to \mathfrak{g}$ defined by $\mathrm{ad}_X(Y) = [X, Y]$.

For our particular situation where we identify the space M of isomorphic frames of type $(n_1, \ldots, n_r)$ with a coset space as in section 1.2.3, we will take G to be U_n and H to be the subgroup defined in section 1.2.3. Thus $\mathfrak{g}$ is just the set of $n \times n$ skew-hermitian matrices, and $\mathfrak{h}$ consists of the block diagonal skew-hermitian matrices. Note that throughout this chapter $\mathcal{E}$ is a fixed frame.

3.1 Riemannian metric

We now proceed to define the natural Riemannian metric on M derived from that on U_n.

The embedding $U_n \subset \mathbb{C}^{n^2} \cong \mathbb{R}^{2n^2}$ induces a bi-invariant Riemannian metric on U_n; if $V \in U_n$ and X, Y lie in the tangent space $T_V U_n = V\mathfrak{g}$ of U_n at V, then

$$\langle X, Y \rangle_V = \operatorname{Re}\operatorname{Tr} Y^* X. \tag{3.2}$$

(Recall that a metric is bi-invariant if for any $a, b \in G$ and $X, Y \in T_b G$ we have

$$\langle X, Y \rangle_b = \langle (dL_a)_b X, (dL_a)_b Y \rangle_{ab} = \langle (dR_a)_b X, (dR_a)_b Y \rangle_{ba}, \tag{3.3}$$

that is, both L_a and R_a are isometries for any $a \in G$).

The geodesics through a unitary $U \in U_n$ are given by the curves $U \exp(tX)$, where X is skew-hermitian. The arclength distance $d(I, U)$ between I and U is the distance along the shortest geodesic $\alpha_X(t) = \exp(tX)$ from I to U, that is,

$$\begin{aligned} d(I, U) &= \inf\{\int_0^1 \sqrt{\langle \alpha_X'(t), \alpha_X'(t) \rangle} dt : X \in \mathfrak{g} \text{ and } \exp(X) = U\} \\ &= \inf\{\|X\|_2 : X \in \mathfrak{g} \text{ and } \exp(X) = U\} \\ &= \sqrt{\sum_k (\arg \lambda_k)^2} \end{aligned} \tag{3.4}$$

where $\{\lambda_k\}$ are the eigenvalues of U and arg takes values in the interval $(-\pi, \pi]$.

This metric on G gives an inner product on $T_e G = \mathfrak{g}$, so we can define

$$\mathfrak{m} = \mathfrak{h}^\perp = \{K \in iM_n^h : \mathcal{E}K = 0\}.$$

One can verify that $\mathfrak{m}$ is invariant under $\mathrm{Ad}(H)$ (in particular $[\mathfrak{h}, \mathfrak{m}] \subset \mathfrak{m}$), so G/H is a reductive homogeneous space with respect to the decomposition $\mathfrak{g} = \mathfrak{h} \oplus \mathfrak{m}$ (see [22, p.343] or [14, p.190]).

From [22, p.151] it follows that $\ker d\pi_e = \mathfrak{h}$ (or more generally, $\ker d\pi_V = dL_V(\mathfrak{h})$ by (3.1)) and so to each $Y \in T_{\hat{e}}M$ there exists a unique $X \in \mathfrak{m}$ such that $d\pi_e(X) = Y$. We denote this isomorphism by $\mu : T_{\hat{e}}M \to \mathfrak{m}$, that is, $\mu(Y) = X$. Note that $d\pi_e \circ \mu$ is the identity map on $T_{\hat{e}}M$, and

$$\mu \circ d\pi_e = \mathcal{E}^{\perp}|_{iM_n^h}. \tag{3.5}$$

The metric on U_n induces the following Riemannian metric on M. Let V be a unitary representing $\hat{V} \in M$ and let $X_1, X_2 \in T_{\hat{V}}M$; we define an inner product on the tangent space of M at $\hat{V}$ in terms of the metric on U_n by

$$\langle X_1, X_2 \rangle_{\hat{V}} = \langle \mu(d\hat{L}_{V^{-1}}X_1), \mu(d\hat{L}_{V^{-1}}X_2) \rangle_e. \tag{3.6}$$

One can check that this gives a well-defined U_n-invariant metric (that is, $\hat{L}_U$ is an isometry for any $U \in U_n$).

3.2 Geodesics and distance

With the metric defined by (3.6), one naturally wonders what the geodesics on M are, and how to compute the Riemannian distance between any two frames. By [11, p.226], the geodesics through $\hat{U} \in G/H$ are precisely the curves $\alpha_X(t) = \pi(U\exp(tX)), X \in \mathfrak{m}$. Translating back into the language of frames, this says that a smooth curve $\mathcal{E}(t)$ with $\mathcal{E}(0) = \mathcal{E}$ is a geodesic iff $\mathcal{E}(t) = \exp(tX)\mathcal{E}\exp(-tX)$ for some $X \in \mathfrak{m}$, which is precisely Kovarik's criterion for geodesics [17]; that is, this coset space geometry and Kovarik's geometry coincide.

The following theorem gives the length for these geodesics and for other paths in M.

Theorem 3.2.1. *Let $\alpha(t)$, $t \in [a, b]$, be a smooth path in M with a lift $U(t)$ in U_n. The length of α is given by*

$$l(\alpha) = \int_a^b \|\mathcal{E}^{\perp}(U^*(t)U'(t))\|_2 \, dt \tag{3.7}$$

where $\|\cdot\|_2$ is the Frobenius norm.

Remark 3.2.2. 1. Observe that, since the length of $U(t)$ in U_n is

$$l(U) = \int_a^b \|U^*(t)U'(t)\|_2 \, dt$$

and $\|\mathcal{E}^{\perp}A\|_2 \le \|A\|_2$ for any $A \in iM_n^h$, the projection π is a contractive map.

2. By [14, Vol I,p.69], for each V in the coset $\alpha(0)$ there exists a unique horizontal lift $V(t)$ in U_n such that $V(0) = V$. (Here a curve $V(t)$ is horizontal iff $V^*(t)V'(t) \in \mathfrak{m}$, that is, $\mathcal{E}(V^*(t)V'(t)) = 0$). Thus the length of $\alpha(t)$ is equal to the length of its horizontal lift in U_n.

3. In particular, for the special case where $\alpha(t)$, $t \in [0,1]$, is a geodesic in M, we can lift $\alpha(t)$ to a geodesic $U(t) = \exp(tX)$ in U_n where $X \in \mathfrak{m}$; thus the length of $\alpha(t)$ is

$$\int_0^1 \|\mathcal{E}^\perp(U^*(t)U(t)X)\|_2\, dt = \|X\|_2,$$

which is just the length of the curve $U(t)$ in U_n.

Proof.

$$\begin{aligned}
l(\alpha) &= \int_a^b \langle \alpha'(t), \alpha'(t)\rangle_{\alpha(t)}^{\frac{1}{2}} dt \\
&= \int_a^b \langle d\pi\, U'(t), d\pi\, U'(t)\rangle_{\hat{U(t)}}^{\frac{1}{2}} dt \\
&= \int_a^b \langle \mu\, d\hat{L}_{U^{-1}(t)} d\pi\, U'(t), \mu\, d\hat{L}_{U^{-1}(t)} d\pi\, U'(t)\rangle_{\hat{e}}^{\frac{1}{2}} dt && \text{by (3.6)} \\
&= \int_a^b \langle \mu\, d\pi\, dL_{U^{-1}(t)} U'(t), \mu\, d\pi\, dL_{U^{-1}(t)} U'(t)\rangle_{\hat{e}}^{\frac{1}{2}} dt && \text{by (3.1)} \\
&= \int_a^b \langle \mathcal{E}^\perp|_{iM_n^h}(U^{-1}(t)U'(t)), \mathcal{E}^\perp|_{iM_n^h}(U^{-1}(t)U'(t))\rangle_{\hat{e}}^{\frac{1}{2}} dt && \text{by (3.5)} \\
&= \int_a^b \|\mathcal{E}^\perp(U^*(t)U'(t))\|_2\, dt
\end{aligned}$$

□

With this proposition in hand, we can compute the distance between any two points of M.

Theorem 3.2.3. *Let d denote the arclength distance on U_n and let d_g denote the arclength distance on U_n/H (the 'g' is for geodesic). If $\hat{U}$ and $\hat{V}$ are two points in U_n/H then*

$$\begin{aligned}
d_g(\hat{U}, \hat{V}) &= \inf_{h \in H} d(U, Vh) \\
&= \inf_{h \in H} \|\ln(U^*Vh)\|_2
\end{aligned}$$

where the branch cut of ln *is the negative real axis.*

Proof.

$$\begin{aligned} d_g(\hat{U}, \hat{V}) &\equiv \inf\{l(\alpha(t)) : \alpha(t) \in U_n/H \text{ is a path joining } \hat{U} \text{ and } \hat{V}\} \\ &\leq \inf_{h\in H} \inf\{l(\beta(t)) : \beta(t) \in U_n \text{ is a path joining } U \text{ and } Vh\} \quad \because\ \pi \text{ is contractive} \\ &= \inf_{h\in H} d(U, Vh). \end{aligned}$$

But $d_g(\hat{U}, \hat{V})$ is also equal to the length of the minimal geodesic joining $\hat{U}$ and $\hat{V}$, and we had shown (see Remark 3.2.2) that this geodesic has the same length as a lift in U_n joining U and Vh for some $h \in H$. Thus we can conclude that

$$\begin{aligned} d_g(\hat{U}, \hat{V}) &= \inf_{h\in H} d(U, Vh) \\ &= \inf_{h\in H} d(I, U^*Vh) && \text{since the metric on } U_n \text{ is bi-invariant} \\ &= \inf_{h\in H} \| \ln(U^*Vh)\|_2 && \text{by (3.4)} \end{aligned}$$

□

Remark 3.2.4. One can optimize the real-valued function on $\mathbb{R}$ given by $x \mapsto d^2(U, Ve^{ix})$ using techniques from elementary calculus to see that the above infimum is necessarily attained at a unitary $h_0 \in H$ for which $\det U^*Vh_0 = 1$ and $-1 \notin \sigma(U^*Vh_0)$. Moreover, the geodesic joining I and U^*Vh_0 in U_n has the same length as the geodesic joining the cosets of H represented by I and U^*V, so $U^*Vh_0 = \exp X$ for some $X \in \mathfrak{m}$. In this case we shall say $\exp X$ is a *geodesic rotation* between $\hat{U}$ and $\hat{V}$; Kovarik [17] uses the term 'direct rotation' instead.

Note that an obvious generalization of d_g is obtained if one replaces the Frobenius norm of $\ln U^*Vh$ by some other unitarily invariant norm.

Chapter 4

Angles between Frames

Although our primary objective is to compare different distances between a pair of frames, we now change our focus slightly and consider sets of angles between two frames. The motivation for this originates from the problem of comparing two subspaces: no matter what distance one uses to measure how far apart two subspaces are, it is but a single number, and so cannot convey the same amount of information contained in the canonical angles between the two subspaces. As for relations between different distances, one can obtain an infinite number of inequalities in one stroke by proving weak majorization relations between different sets of angles. Clearly there is a great deal of potential in such an approach. Moreover, the angles $\Phi(E, F)$ that we shall define between two ordered frames E and F should be more amenable to our geometric intuition of frames as objects based in $\mathbb{C}^n$.

4.1 Definitions of Angles

We begin by investigating quantities which are more closely related to the realization of frames as direct sum decompositions of $\mathbb{C}^n$ into orthogonal subspaces. Let us first consider the case where $\mathcal{E} = \{e_1e_1^*, \ldots, e_ne_n^*\}$ and $\mathcal{F} = \{f_1f_1^*, \ldots, f_nf_n^*\}$ are two minimal frames, so $\mathcal{E}$ and $\mathcal{F}$ can be more or less thought of as unordered orthonormal bases, although they are not so much bases of vectors as bases of lines.

One way of measuring the distance between two lines in $\mathbb{C}^n$ is to use the Fubini-Study distance [13] derived from the usual Euclidean distance; if u, v are unit vectors in $\mathbb{C}^n$, the Fubini-Study distance d_{FS} between the two lines $\mathbb{C}u$ and $\mathbb{C}v$ is defined by

$$d_{FS}(\mathbb{C}u, \mathbb{C}v) = \inf_{\theta} \|u - ve^{i\theta}\|_2.$$

We can use this to define an optimal matching distance d_b between $\mathcal{E}$ and $\mathcal{F}$ by

$$d_b(\mathcal{E},\mathcal{F}) = \inf_{\sigma\in S_n} \sqrt{\sum_{i=1}^{n} d_{FS}^2(\mathbb{C}e_i, \mathbb{C}f_{\sigma(i)})}. \tag{4.1}$$

Note that if $U = (e_1|\ldots|e_n)$ and $V = (f_1|\ldots|f_n)$ then

$$d_b^2(\mathcal{E},\mathcal{F}) = \inf_{h\in H} \|U - Vh\|_2^2.$$

This can clearly be generalized to other unitarily invariant norms and to more general frames.

Proposition 4.1.1. *Let M be the space of isomorphic frames of a fixed type. If $\mathcal{E}$ and $\mathcal{F}$ are two frames in M which are identified with the cosets of H represented by U and V respectively, then for any unitarily invariant norm $\|\cdot\|$,*

$$d(\mathcal{E},\mathcal{F}) = \inf_{h\in H} \|U - Vh\| = \inf_{h\in H} \|I - U^*Vh\| \tag{4.2}$$

defines a metric on M.

Proof. Clearly d is non-degenerate. To see that d is symmetric and that the triangle inequality holds, note that, due to the unitary invariance of the norm and the fact that H is a group,

$$\inf_{h\in H} \|U - Vh\| = \inf_{g,h\in H} \|Ug - Vh\|.$$

□

Remark 4.1.2. The infimum is in general attained at different values of $h \in H$ for different unitarily invariant norms; in the particular case when the norm in (4.2) is the Frobenius norm, Davis [6] showed that the infimum is attained when $E_iU^*VhE_i \geq 0$ for each i, or equivalently, $\mathcal{E}(U^*Vh) \geq 0$. For more, see section 4.2.

Note that this family of distances depends on the spectra of U^*Vh, and so is based in M_n, as opposed to our intent of finding a distance based in $\mathbb{C}^n$. Returning to the special case of minimal frames, an alternative approach to using the Fubini-Study metric to measure the distance between two lines is to use the angle between the lines. One would probably argue that this approach is better because it is a more intrinsic measure of how far apart two lines are, and allows the possibility of geodesics, just as the arclength distance on the sphere instead of the Euclidean distance is preferable.

To use this idea for frames which are not necessarily minimal, we need to generalize the notion of an angle between a pair of lines to a set of angles between a pair of subspaces. It is well known that for any pair of subspaces of the same finite dimension k, there is a natural set of canonical angles between them (see for example [4, 7]).

Definition 4.1.3. Let P and Q be projections of the same rank k. The canonical angles between the subspaces $\operatorname{Ran} P$ and $\operatorname{Ran} Q$ will be denoted by $\Theta(P,Q)$ and are given by

$$\Theta(P,Q) = \arcsin s(Q^{\perp}P|_{\operatorname{Ran} P}) = \arcsin s(P^{\perp}Q|_{\operatorname{Ran} Q}).$$

Remark 4.1.4. Note that the definition is symmetric in P and Q, and the canonical angles all lie in the interval $[0, \frac{\pi}{2}]$. We may also characterize the canonical angles by

$$\cos^2 \Theta(P,Q) = \lambda(PQP|_{\operatorname{Ran} P}) = \lambda(QPQ|_{\operatorname{Ran} Q}).$$

Henceforth, we will abuse notation by having $\Theta(P,Q)$ represent both a set of k elements and also a vector of k angles, arranged in decreasing order. (In fact, all sets of angles in this work will suffer from this dual personality; the context should eliminate any confusion).

Since an ordered frame is just a collection of projections in some predetermined order, we can define a set of angles $\Phi(E,F)$ between two ordered frames E, F by using the angles between pairs of corresponding projections. The quantity $\|\Phi(E,F)\|$ (for each symmetric gauge function) should then serve as a useful measure of how far apart E and F are.

Definition 4.1.5. Let $E = (E_1, \ldots, E_r)$ and $F = (F_1, \ldots, F_r)$ be two ordered frames of the same type $(n_1, \ldots, n_r)$. (Thus rank E_i = rank $F_i = n_i$ and $\sum_{i=1}^{r} n_i = n$.) We define a set of angles $\Phi(E,F)$ between E and F by

$$\Phi(E,F) = \cup_{i=1}^{r} \Theta(E_i, F_i).$$

Remark 4.1.6. Since E and F are isomorphic, there exists a unitary U which intertwines E and F, i.e., $UE_i = F_iU$ for all i. Thus $E_iF_iE_i = E_iUE_iU^*E_i$, so $\cos\Theta(E_i, F_i)$ consists of the singular values of $E_iUE_i|_{\operatorname{Ran} E_i}$. If we write U in block matrix form with respect to $\mathbb{C}^n = \oplus_{i=1}^{r} \operatorname{Ran} E_i$ so that U has (i,j)-block-entry $U_{ij} = E_iUE_j|_{\operatorname{Ran} E_j}$, it follows that

$$\cos \Phi(E,F) = \cup_{i=1}^{r} s(U_{ii}) = s(\mathcal{E}U).$$

One might wonder if the definition of $\Phi(E,F)$ can be extended to unordered frames; unfortunately, there is no a priori pairing of the constituent projections of two unordered frames in general, and there seems to be no way to resolve this difficulty. For examples illustrating the problem, see the next section.

However, one can still define a set of angles between $\mathcal{E}$ and $\mathcal{F}$, albeit from a rather different viewpoint; since $\mathcal{E}$ and $\mathcal{F}$ can also be viewed as projections in $\mathcal{B}(M_n)$, it makes sense to speak of the canonical angles $\Theta(\mathcal{E},\mathcal{F})$ (so $\cos^2\Theta(\mathcal{E},\mathcal{F}) = \lambda(\mathcal{E}\mathcal{F}\mathcal{E}|_{\mathrm{Ran}\,\mathcal{E}})$). Note that the number of angles in $\Theta(\mathcal{E},\mathcal{F})$, if rank $E_i = n_i$, is equal to $\dim\mathcal{E} = \sum_{i=1}^r n_i^2$. In order to compare $\Phi(E,F)$ with $\Theta(\mathcal{E},\mathcal{F})$, the two sets should have the same number of elements; however, $\Phi(E,F)$ only contains n angles. To this end we introduce the following variants of $\Phi(E,F)$.

Definition 4.1.7. Let $E = (E_1,\ldots,E_r)$ and $F = (F_1,\ldots,F_r)$ be two ordered frames of the same type $(n_1,\ldots,n_r)$. (Thus rank E_i = rank $F_i = n_i$ and $\sum_{i=1}^r n_i = n$.) Denote the angles in $\Theta(E_i,F_i)$ by ϕ_{ij}, $1 \le j \le n_i$. Thus

$$\Phi(E,F) = \{\phi_{ij} : 1 \le i \le r, 1 \le j \le n_i\} \in \mathbb{R}^n.$$

We define two new sets of angles $\Phi_0(E,F)$ and $\Phi_+(E,F)$ by

$$\Phi_0(E,F) = \{\phi_{ij} \text{ with multiplicity } n_i \ : 1 \le i \le r, 1 \le j \le n_i\} \in \mathbb{R}^{\sum_i n_i^2},$$
$$\Phi_+(E,F) = \{\phi_{ij} + \phi_{ik} : 1 \le i \le r, 1 \le j,k \le n_i\} \in \mathbb{R}^{\sum_i n_i^2}.$$

Note that we shall simply write Θ for $\Theta(\mathcal{E},\mathcal{F})$ when there is no chance of confusion (and similarly for Φ, Φ_0, Φ_+).

Having introduced all the main players, let us summarize the quantities we wish to compare.

1. Frames are viewed as pinchings in $\mathcal{B}(M_n)$. We have angles $\Theta(\mathcal{E},\mathcal{F})$ associated with the distance $\|\mathcal{E}-\mathcal{F}\| = \|\sin\Theta \oplus \sin\Theta\|$. (See (2.2) or [4] for the preceding equality.)

2. Frames are viewed as cosets of H in U_n. We have the distance $\inf_{h\in H}\|U - Vh\|$ and $\inf_{h\in H}\|\ln U^*Vh\|$ (a generalization of the Riemannian distance); if the eigenvalues of U^*Vh are $e^{i\alpha_j}$, we can think of α_j as angles between the frames represented by U and V.

3. Frames are viewed as collections of orthogonal subspaces. We have angles Φ, Φ_0, Φ_+; the symmetric gauge functions applied to these angles will measure how far apart two frames are.

We conclude this section by noting the following fact.

Proposition 4.1.8. $\Phi_+(E,F) \prec 2\Phi_0(E,F)$.

Proof. By Proposition 1.3.9 it suffices to show that, for each i,

$$\{\phi_{ij} + \phi_{ik} : 1 \leq j, k \leq n_i\} \prec \{2\phi_{ij} \text{ with multiplicity } n_i : 1 \leq j \leq n_i\}.$$

Thus we wish to show that

$$\{x_j + x_k : 0 \leq j, k \leq n-1\} \prec \{2x_j \text{ with multiplicity } n : 0 \leq j \leq n-1\}.$$

Let x_+ be the vector in $\mathbb{R}^{n^2}$ whose jth coordinate is $x_{[j/n]} + x_{j \bmod n}$, and let x_0 be the vector in $\mathbb{R}^{n^2}$ whose jth coordinate is $x_{[j/n]}$. Here j runs from 0 to $n^2 - 1$, $[j/n]$ is the greatest integer less than or equal to j/n, and $j \bmod n$ takes values in $\{0, 1, \ldots, n-1\}$. We wish to show $x_+ \prec 2x_0$.

Define a permutation σ on the n^2 elements $\{0, 1, \ldots, n^2-1\}$ by $\sigma(an+b) = a+nb$, where $a, b \in \{0, 1, \ldots, n-1\}$. We identify σ with the $n^2 \times n^2$ matrix which has $(i+1, j+1)$ entry equal to one if $j = \sigma(i)$ and zero otherwise. Let $S = \frac{1}{2}(I + \sigma)$. Then S is doubly stochastic and $Sx_0 = \frac{1}{2}x_+$, so $x_+ \prec 2x_0$, as desired.

□

4.2 Unitaries intertwining frames

This rather pessimistic section contains examples which illustrate two negative results: there is no canonical best way to pair the projections of two isomorphic (unordered) frames in general, and there is no canonical best way to rotate from one frame to another.

Note that the angles $\Phi(E,F)$ are only defined between ordered frames $E = (E_1, \ldots, E_r)$ and $F = (F_1, \ldots, F_r)$; one may wonder if it is possible to extrapolate the definition of $\Phi(E,F)$ to define angles between the unordered frames $\mathcal{E} = \{E_1, \ldots, E_r\}$ and $\mathcal{F} = \{F_1, \ldots, F_r\}$ by finding a 'best' pairing of the projections E_i with F_i, in the sense of making the associated angles small? More precisely, given a permutation $\sigma \in S_r$, let F_σ be the ordered frame $(F_{\sigma(1)}, \ldots, F_{\sigma(r)})$ and write Φ_σ for $\Phi(E, F_\sigma)$ (note that σ must permute projections of the same rank). Can we find a permutation σ such that $\Phi_\sigma \prec_w \Phi_\rho$ (or maybe even $\Phi_\sigma \leq \Phi_\rho$) for all permutations ρ? If $\|\Phi(E,F)\|_\infty \leq \frac{\pi}{4}$ then the answer is yes (to the strong assertion); otherwise the answer is no in general.

Proposition 4.2.1. *If $\|\Phi(E,F)\|_\infty \leq \frac{\pi}{4}$ then $\Phi(E,F) \leq \Phi_\rho$ for all permutations ρ.*

Proof. Let U be a unitary which satisfies $UE_iU^* = F_i$ for all i. Following the notation in Remark 4.1.6 we can write U as a block matrix with (i,j)-block-entry U_{ij}. Since $\cos\Phi(E,F) = \cup_{i=1}^r s(U_{ii})$, the hypothesis $\|\Phi(E,F)\|_\infty \le \frac{\pi}{4}$ implies that for each i, all of the singular values of U_{ii} are larger than $\frac{1}{\sqrt{2}}$, or equivalently, $U_{ii}U_{ii}^* \ge \frac{1}{2}E_i$. Since U is unitary, it follows that

$$\sum_{j\neq i} U_{ij}U_{ij}^* = E_i - U_{ii}U_{ii}^* \le E_i - \frac{1}{2}E_i = \frac{1}{2}E_i \le U_{ii}U_{ii}^* \tag{4.3}$$

for each i.

Now suppose $\rho \in S_r$ permutes projections of the same rank. Let V be the unitary with (i,j)-block-entry equal to $U_{i\rho(j)}$; it follows that $VE_iV^* = F_{\rho(i)}$. Thus $\cos\Phi(E,F_\rho) = \cup_{i=1}^r s(U_{i\rho(i)})$. But (4.3) says that $U_{i\rho(i)}U_{i\rho(i)}^* \le U_{ii}U_{ii}^*$ for each i, so $\cos\Phi(E,F_\rho) \le \cos\Phi(E,F)$. Hence $\Phi(E,F) \le \Phi_\rho$ as claimed.

□

This shows that if all the angles of $\Phi(E,F)$ are less than $\frac{\pi}{4}$, then any other pairing results in larger angles. The following example shows that the bound of $\frac{\pi}{4}$ is necessary for the above proposition.

Example 4.2.2. Let $r = 2$ so we can write $E_1 = P$, $E_2 = P^\perp$. Similarly, we write $F_1 = Q, F_2 = Q^\perp$. We will assume rank P = rank $P^\perp$, so that there are exactly two ways to pair the projections of $\mathcal{E}$ and $\mathcal{F}$; that is, we can compare $E = (P, P^\perp)$ to $F = (Q, Q^\perp)$ and also to $\tilde{F} = (Q^\perp, Q)$.

Suppose the canonical angles $\Theta(P,Q)$ between P and Q consist of k angles of $\frac{\pi}{4} - \delta$ and l angles of $\frac{\pi}{4} + \epsilon$, where $0 < \delta < \epsilon < \frac{\pi}{4}$. Thus the canonical angles between P and $Q^\perp$ comprise k angles of $\frac{\pi}{4} + \delta$ and l angles of $\frac{\pi}{4} - \epsilon$.

Note that since rank P = rank $P^\perp$, $\Theta(P,Q) = \Theta(P^\perp, Q^\perp)$ and $\Theta(P, Q^\perp) = \Theta(P^\perp, Q)$. It follows that

$$\|\Phi(E,F)\|_\infty - \|\Phi(E,\tilde{F})\|_\infty = (\frac{\pi}{4} + \epsilon) - (\frac{\pi}{4} + \delta) > 0$$

while for each $p \in [1,\infty)$,

$$\|\Phi(E,F)\|_p^p - \|\Phi(E,\tilde{F})\|_p^p = 2l[(\frac{\pi}{4} + \epsilon)^p - (\frac{\pi}{4} - \epsilon)^p] + 2k[(\frac{\pi}{4} - \delta)^p - (\frac{\pi}{4} + \delta)^p]$$

which can be made less than zero by an appropriate choice of k and l.

This shows that if $\|\Phi(E,F)\|_\infty > \frac{\pi}{4}$, one does not have $\Phi(E,F) \prec_w \Phi(E,F_\rho)$ in general. In particular, any 'best' choice of pairing projections will depend in general on which unitarily invariant norm we use to measure how big the angles are.

The same difficulty exists for minimal frames.

Example 4.2.3. Let $\mathcal{E}, \mathcal{F}$ be two minimal frames with $F_i = UE_iU^*$, where U is the $(n+1) \times (n+1)$ orthogonal matrix with entries

$$U_{ij} = \begin{cases} \frac{1}{\sqrt{n}}, & \text{if } i = n+1 \text{ or } j = n+1 \text{ and } i \neq j; \\ 0, & \text{if } i = j = n+1; \\ \frac{n-1}{n}, & \text{if } i = j < n+1; \\ -\frac{1}{n}, & \text{otherwise.} \end{cases}$$

In matrix form,

$$U = \begin{pmatrix} \frac{n-1}{n} & -\frac{1}{n} & \cdots & -\frac{1}{n} & \frac{1}{\sqrt{n}} \\ -\frac{1}{n} & \ddots & & \vdots & \vdots \\ \vdots & & \ddots & -\frac{1}{n} & \vdots \\ -\frac{1}{n} & \cdots & -\frac{1}{n} & \frac{n-1}{n} & \frac{1}{\sqrt{n}} \\ \frac{1}{\sqrt{n}} & \cdots & \cdots & \frac{1}{\sqrt{n}} & 0 \end{pmatrix}.$$

If ρ is a permutation in S_{n+1}, then $\cos\Phi(E, F_\rho) = \{|U_{i\rho(i)}| : 1 \leq i \leq n+1\}$. Thus, there are clearly only two candidates for an optimal pairing of projections (in the sense of minimizing the angles): ρ is either the identity permutation or the transposition switching n and $n+1$. Let γ and δ denote the angles corresponding to these two cases respectively; thus $\cos\gamma$ is given by the diagonal entries of U, and, if V is the unitary obtained by switching the last two columns of U, $\cos\delta$ is given by the diagonal entries of V. Hence

$$\cos\gamma = (\frac{n-1}{n}, \ldots, \frac{n-1}{n}, 0),$$
$$\cos\delta = (\frac{n-1}{n}, \ldots, \frac{n-1}{n}, \frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}}).$$

Clearly for any $p \in [1, \infty)$ one can make

$$||\delta||_p > ||\gamma||_p$$

by choosing n sufficiently large; however

$$||\delta||_\infty < ||\gamma||_\infty$$

for any choice of n, so once again a 'best' pairing depends on the choice of norm used to measure the size of the angles.

Due to the lack of a natural way to match the projections of two frames, one would suspect that there is not a uniformly best way to rotate from one frame to another. First let us clarify what is meant by rotating from one frame to another.

Definition 4.2.4. Let $E = (E_1, \dots, E_r)$ and $F = (F_1, \dots, F_r)$ be two isomorphic ordered frames, and let $\mathcal{E}$ and $\mathcal{F}$ denote the corresponding unordered frames. A unitary U is said to *intertwine* E and F if $UE_i = F_iU$ for all i. We say U intertwines $\mathcal{E}$ and $\mathcal{F}$ if there exists a permutation $\sigma \in S_r$ for which $UE_i = F_{\sigma(i)}U$ for all i (equivalently, $\phi_U(\mathcal{E}) = \mathcal{F}$).

A natural question is which unitary, of all those intertwining two frames, is closest to the identity. The prototype of the type of result we would ideally like is the following proposition from [7]:

Theorem 4.2.5 (Davis). *Let P and Q be two projections of the same rank. Let U be a unitary satisfying:*

1. $UP = QU$.
2. *If U is written in block matrix form with respect to the direct sum decomposition $\mathcal{H} = P\mathcal{H} \oplus P^{\perp}\mathcal{H}$ as*
$$\begin{pmatrix} C_0 & -S_1 \\ S_0 & C_1 \end{pmatrix}$$
then $C_0 \geq 0$, $C_1 \geq 0$, $S_1 = S_0^*$.

(The unitary U is called a direct rotation *from P to Q).*

Then for every unitarily invariant norm, the minimum of $\|(I - V^*)(I - V)\|$ over all unitaries V satisfying $VP = QV$ is attained when $V = U$.

Remark 4.2.6. The result is equivalent to saying that for every Q-norm, the minimum of $\|I - V\|$ is attained when $V = U$.

One may well wonder if we could extend this result about subspaces to an analogous result about frames. Can one find a unitary U intertwining two frames $\mathcal{E}$ and $\mathcal{F}$ for which
$$\inf\{\|I - V\| : V \text{ intertwines } \mathcal{E} \text{ and } \mathcal{F}\}$$
is attained at U for all Q-norms? The following example shows that such a generalization is unlikely.

Example 4.2.7. Let $U = I - 2J_n$, so U is the $n \times n$ symmetric orthogonal matrix

$$\begin{pmatrix} \frac{n-2}{n} & -\frac{2}{n} & \cdots & \\ -\frac{2}{n} & \frac{n-2}{n} & \ddots & \\ \vdots & \ddots & \ddots & \\ & & & \frac{n-2}{n} \end{pmatrix}.$$

The only eigenvalues of U are 1 (with multiplicity $n-1$) and -1 (with multiplicity 1). Let $\mathcal{E}$ be the minimal frame comprising the projections $e_i e_i^*$, and let $\mathcal{F}$ be the minimal frame of projections $Ue_ie_i^*U^*$.

Note that the set of unitaries intertwining E and F is precisely $\{Uh : h \in H\}$, where H consists of those unitaries which are products of a diagonal unitary and a permutation.

Since

$$\|I - Uh\|_2^2 = \mathrm{Tr}(I - Uh)^*(I - Uh) = 2 - 2\,\mathrm{Re}\,\mathrm{Tr}\,Uh,$$

$\|I - Uh\|_2$ is minimized when $|\mathrm{Tr}\,Uh|$ is maximized. As $|\mathrm{Tr}\,Uh|$ is clearly maximized over $h \in H$ when $h = I$ it follows that

$$\|I - U\|_2 = \inf_{h \in H} \|I - Uh\|_2.$$

On the other hand

$$2 = \|I - U\| = \sup_{h \in H} \|I - Uh\|.$$

This shows that we cannot find a unitary intertwining $\mathcal{E}$ and $\mathcal{F}$ which minimizes $\|I - V\|$ for all Q-norms. This is in spite of the fact that $\mathcal{E}$ and $\mathcal{F}$ are quite close; the angles between $\mathcal{E}$ and $\mathcal{F}$ are all $\arccos \frac{n-2}{n}$, which tend to zero as n becomes large. Thus the non-existence of an optimal unitary for all Q-norms occurs for ordered frames as well.

Remark 4.2.8. In general, the minimum of $\|I - V\|_2$ over unitaries V intertwining two frames $\mathcal{E}$ and $\mathcal{F}$ is attained at a unitary U which satisfies

$$\phi_U(\mathcal{E}) = \mathcal{F}, \text{ and}$$
$$\mathcal{E}U \geq 0.$$

This unitary was investigated by Davis in [6] and also by Kovarik and Sherif in [16, 25, 26]; we shall follow Kovarik's notation and call U a *balanced transformation* between $\mathcal{E}$ and $\mathcal{F}$. Similarly, if U intertwines two ordered frames E and F, and $\mathcal{E}U \geq 0$, we say U is a balanced transformation between E and F.

4.3 Some Inequalities

Proposition 4.3.1. *Let U be a unitary with eigenvalues $e^{i\alpha_j}$. Let $\mathcal{E}$ be a pinching, and let $\cos\phi$ denote the singular values of $\mathcal{E}U$, where $0 \le \phi \le \frac{\pi}{2}$. Then $\sin^2\frac{\phi}{2} \prec_w \sin^2\frac{\alpha}{2}$.*

Proof. Recall that $\lambda(\operatorname{Re} A) \le s(A)$ for any matrix A (for instance, see [4, Chapter 3]). Taking $A = \mathcal{E}U$ gives

$$\begin{aligned}
\sin^2\frac{\phi}{2} &= \frac{1-\cos\phi}{2} = \frac{1-s(\mathcal{E}U)}{2} \\
&\le \frac{1-\lambda(\operatorname{Re}\mathcal{E}U)}{2} = \frac{1}{2}\lambda(I-\operatorname{Re}\mathcal{E}U) \\
&= \frac{1}{2}\lambda(\mathcal{E}\operatorname{Re}(I-U)) \prec \frac{1}{2}\lambda(\operatorname{Re}(I-U)) \\
&= \frac{1-\cos\alpha}{2} = \sin^2\frac{\alpha}{2}
\end{aligned}$$

as required. □

Remark 4.3.2.

1. We do not have $\sin^2\phi \prec_w \sin^2\alpha$ in general. Nor do we have $\sin\frac{\phi}{2} \prec_w \sin\frac{\alpha}{2}$. This is regardless of any bounds we might impose on ϕ or α. To see this, consider the unitary

$$U = \begin{pmatrix} d & -\sqrt{d-d^2} & 1-d & \sqrt{d-d^2} \\ \sqrt{d-d^2} & d & -\sqrt{d-d^2} & 1-d \\ 1-d & \sqrt{d-d^2} & d & -\sqrt{d-d^2} \\ -\sqrt{d-d^2} & 1-d & \sqrt{d-d^2} & d \end{pmatrix}$$

where $d \in [0,1]$, and take $\mathcal{E}$ to be the pinching onto the diagonal with respect to the standard basis. Note that the eigenvalues of U are given by

$$(1, 1, 2d-1-2i\sqrt{d(1-d)}, 2d-1+2i\sqrt{d(1-d)}),$$

with corresponding orthogonal eigenvectors $(0,1,0,1)$, $(1,0,1,0)$, $(i,-1,-i,1)$, and $(-i,-1,i,1)$.

2. Since the function $(\arcsin\sqrt{x})^p$ is convex and increasing for any $p \ge 2$, it follows by Theorem 1.3.8 that $\phi^p \prec_w \alpha^p$ for any $p \ge 2$. That this does not necessarily hold for $p < 2$ may be seen by considering the unitary U above with d sufficiently close to 1.

Corollary 4.3.3. *Let E and F be ordered frames of the same type. Then*

$$\|\sin\frac{\Phi(E,F)}{2}\| \leq \frac{1}{2}\inf\{\|I-U\| : U \text{ intertwines } E \text{ and } F\}$$

for any Q-norm.

Also

$$\|\Phi(E,F)\|_p \leq \inf\{\|\ln U\|_p : U \text{ intertwines } E \text{ and } F\}$$

for all $p \geq 2$.

Proof. Wolog represent E and F by the unitaries I and V respectively. Then a unitary U intertwines E and F iff $U = Vh$ for some block diagonal (with respect to $\ominus \operatorname{Ran} E_i\mathcal{H}$) unitary h. If the eigenvalues of U are $e^{i\alpha_j}$, then the singular values of $I-U$ and $\ln U$ are $2\sin\frac{\alpha_j}{2}$ and $|\alpha_j|$, respectively. Since

$$s(\mathcal{E}U) = s(\mathcal{E}(Vh)) = s((\mathcal{E}V)h) = s(\mathcal{E}V) = \cos\Phi(E,F)$$

by Remark 4.1.6, the assertions follow from the preceding proposition and remark. □

Remark 4.3.4. We can minimize over all possible pairings of projections to obtain a similar result for unordered frames.

Proposition 4.3.5. *Let V be a unitary matrix. Then*

$$\inf_{h\in H}\|I - Vh\| \leq \inf_{h\in H}\|\ln Vh\| \tag{4.4}$$

for any unitarily invariant norm.

Proof. It suffices to show that $\|I-U\| \leq \|\ln U\|$ for any unitary U. Let U be a unitary with eigenvalues $e^{i\alpha_j}$. The singular values of $\ln U$ are $|\alpha_j|$, while the singular values of $I-U$ are $2|\sin\frac{\alpha_j}{2}|$. Since $2|\sin\frac{\alpha_j}{2}| \leq 2|\frac{\alpha_j}{2}| = |\alpha_j|$, the proposition follows. □

Remark 4.3.6. Since the difference between $2\sin\frac{\alpha}{2}$ and α is of order α^3, the proof shows that the difference between $\inf_{h\in H}\|I - Vh\|$ and $\inf_{h\in H}\|\ln Vh\|$ is of order $(\inf_{h\in H}\|I - Vh\|)^3$.

In the particular case of the Frobenius norm, the infimum on the left hand side of (4.4) is attained when Vh is a balanced transformation, while the infimum on the right hand side is attained when Vh is a geodesic rotation, so we essentially recover the estimate of Kovarik and Sherif [17, 25] which asserts that the balanced transformation and geodesic rotation are cubically close.

4.4 2-frames

In the special case where $\mathcal{E}, \mathcal{F}$ are isomorphic 2-frames we possess considerably more information than in the general case; thus it is fruitful to examine this case separately. For this section, we will write $E = (P, P^{\perp})$ and $F = (Q, Q^{\perp})$, and we will assume wolog $\operatorname{rank} P = \operatorname{rank} Q = k \leq \frac{n}{2}$. The following proposition gives us $\Theta(\mathcal{E}, \mathcal{F})$ in terms of $\Theta(P, Q)$.

Proposition 4.4.1. *Let $\theta_1 \geq \cdots \geq \theta_k$ be the canonical angles between P and Q. Then the angles in $\Theta(\mathcal{E}, \mathcal{F})$ consist of:*

1. *θ_i with multiplicity $2(n-2k)$ for each $i = 1, \ldots, k$*
2. *$|\theta_i - \theta_j|$ for each $i, j = 1, \ldots, k$*
3. *$\min(\theta_i + \theta_j, (\frac{\pi}{2} - \theta_i) + (\frac{\pi}{2} - \theta_j))$ for each $i, j = 1, \ldots, k$*
4. *0 with multiplicity $(n-2k)^2$*

Remark 4.4.2. Note that if $n = 2k$, the above list of angles remains unchanged if we substitute $\frac{\pi}{2} - \theta_i$ for θ_i. This is not surprising, for $n = 2k$ implies that rank P = rank $Q^{\perp}$, so we could just as well pair P with $Q^{\perp}$ and ask for $\Theta(\mathcal{E}, \mathcal{F})$ in terms of $\Theta(P, Q^{\perp})$. Since the angles in $\Theta(P, Q^{\perp})$ are precisely $\{\frac{\pi}{2} - \theta : \theta \in \Theta(P, Q)\}$, this explains the noted invariance.

Proof. We can choose an orthonormal basis (for example, see [4, Chapter 7]) such that, with respect to this basis, the block matrices of P and Q are

$$P = \begin{pmatrix} I & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, Q = \begin{pmatrix} C^2 & SC & 0 \\ SC & S^2 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

where C, S are the diagonal matrices

$$C = \begin{pmatrix} \cos\theta_1 & & & \\ & \cos\theta_2 & & \\ & & \ddots & \\ & & & \cos\theta_k \end{pmatrix}, S = \begin{pmatrix} \sin\theta_1 & & & \\ & \sin\theta_2 & & \\ & & \ddots & \\ & & & \sin\theta_k \end{pmatrix}$$

respectively. Note that the diagonal block entries of P and Q have dimensions k,k, and $n-2k$.

Since the canonical angles between $\mathcal{E}$ and $\mathcal{F}$ satisfy $\sin^2 \Theta(\mathcal{E}, \mathcal{F}) = \lambda(\mathcal{E}\mathcal{F}^{\perp}\mathcal{E}|_{\operatorname{Ran}\mathcal{E}})$, it suffices to compute the eigenvalues of $\mathcal{E}\mathcal{F}^{\perp}\mathcal{E}$ (as an operator on $\operatorname{Ran}\mathcal{E}$). Note

$$\mathcal{F}^{\perp}A = A - \mathcal{F}A = QA + AQ - 2QAQ.$$

Let $A \in \operatorname{Ran}\mathcal{E}$; writing all matrices in block form, we have $A = \begin{pmatrix} Z & 0 & 0 \\ 0 & W & X \\ 0 & Y & T \end{pmatrix}$.
A straightforward computation shows that

$$\mathcal{E}\mathcal{F}^{\perp}\mathcal{E}A = \begin{pmatrix} C^2Z+ZC^2-2C^2ZC^2-2SCWSC & 0 & 0 \\ 0 & S^2W+WS^2-2S^2WS^2-2SCZSC & S^2X \\ 0 & YS^2 & 0 \end{pmatrix}.$$

Let $E^{ij} = e_i e_j^*$ be the matrix with a one in the (i,j) position and zeros elsewhere. It follows that $\mathcal{E}\mathcal{F}^{\perp}\mathcal{E}$ has the following eigenvectors in $\operatorname{Ran}\mathcal{E}$:

1. $\begin{pmatrix} 0 & & \\ & 0 & \\ & & E^{ij} \end{pmatrix}$ with eigenvalue 0 for each $1 \le i, j \le n-2k$.
2. $\begin{pmatrix} 0 & & \\ & 0 & E^{ij} \\ & 0 & \end{pmatrix}$ with eigenvalue $\sin^2\theta_i$ for each $1 \le i \le k, 1 \le j \le n-2k$.
3. $\begin{pmatrix} 0 & & \\ & 0 & \\ & E^{ij} & 0 \end{pmatrix}$ with eigenvalue $\sin^2\theta_j$ for each $1 \le i \le n-2k, 1 \le j \le k$.
4. $\begin{pmatrix} E^{ij} & & \\ & E^{ij} & \\ & & 0 \end{pmatrix}$ with eigenvalue $\sin^2(\theta_i - \theta_j)$ for each $1 \le i, j \le k$.
5. $\begin{pmatrix} E^{ij} & & \\ & -E^{ij} & \\ & & 0 \end{pmatrix}$ with eigenvalue $\sin^2(\theta_i + \theta_j)$ for each $1 \le i, j \le k$.

The eigenvalues for (4) and (5) are evident if we note that

$$\begin{aligned} &\cos^2\theta_j + \cos^2\theta_i - 2\cos^2\theta_i\cos^2\theta_j \pm 2\sin\theta_i\cos\theta_i\sin\theta_j\cos\theta_j \\ =&\cos^2\theta_j(1-\cos^2\theta_i) + \cos^2\theta_i(1-\cos^2\theta_j) \pm 2\sin\theta_i\cos\theta_i\sin\theta_j\cos\theta_j \\ =&\cos^2\theta_j\sin^2\theta_i + \cos^2\theta_i\sin^2\theta_j \pm 2\sin\theta_i\cos\theta_i\sin\theta_j\cos\theta_j \\ =&(\cos\theta_j\sin\theta_i \pm \cos\theta_i\sin\theta_j)^2 \\ =&\sin^2(\theta_i \pm \theta_j). \end{aligned}$$

By noting that $\sin^2\Theta(\mathcal{E},\mathcal{F}) = \sigma(\mathcal{E}\mathcal{F}^{\perp}\mathcal{E})$ and that all angles in $\Theta(\mathcal{E},\mathcal{F})$ are between 0 and $\frac{\pi}{2}$, the proposition follows.

□

Since $\Phi(E,F) = \Theta(P,Q) \cup \Theta(P^{\perp},Q^{\perp})$, and $\Theta(P^{\perp},Q^{\perp})$ just consists of the same angles as $\Theta(P,Q)$ together with $n-2k$ zeros (recall that we've assumed $k \le \frac{n}{2}$), this proposition allows us to derive a number of relations between $\Phi(E,F)$ and $\Theta(\mathcal{E},\mathcal{F})$.

Theorem 4.4.3. *If E and F are isomorphic ordered 2-frames, $\Theta(\mathcal{E},\mathcal{F}) \le \Phi_+(E,F)$. Moreover, if $\|\Phi(E,F)\| \le \frac{\pi}{4}$ for the bound norm $\|\cdot\|$, then $\Phi_0(E,F) \prec_w \Theta(\mathcal{E},\mathcal{F})$.*

Proof. Let $\alpha_1, \ldots, \alpha_k$ denote the angles between P and Q. As noted, the angles between $P^\perp$ and $Q^\perp$ are just $\Theta(P,Q)$ together with $n-2k$ zeros. Hence $\Phi_+(E,F)$ is the union of the four sets of angles

1. $\{\alpha_i + \alpha_j : 1 \le i,j \le k\}$,
2. $\{\alpha_i + \alpha_j : 1 \le i,j \le k\}$,
3. $\{\alpha_i$ with multiplicity $2(n-2k) : 1 \le i \le k\}$,
4. $\{0$ with multiplicity $(n-2k)^2\}$,

whereas, by Proposition 4.4.1, $\Theta(\mathcal{E},\mathcal{F})$ is the union of the four sets of angles

1. $\{\min(\alpha_i + \alpha_j, \pi - (\alpha_i + \alpha_j) : 1 \le i,j \le k\}$,
2. $\{|\alpha_i - \alpha_j| : 1 \le i,j \le k\}$,
3. $\{\alpha_i$ with multiplicity $2(n-2k) : 1 \le i \le k\}$,
4. $\{0$ with multiplicity $(n-2k)^2\}$.

Comparing corresponding sets of angles of $\Phi_+(E,F)$ and $\Theta(\mathcal{E},\mathcal{F})$ gives the first statement.

For the second statement, note that $\Phi_0(E,F)$ comprises n copies of α_i, $1 \le i \le k$, together with $(n-2k)(n-k)$ zeros. We can rewrite $\Phi_0(E,F)$ as the union of the four sets of angles

1. $\{\alpha_i$ with multiplicity $k : 1 \le i \le k\}$,
2. $\{\alpha_i$ with multiplicity $k : 1 \le i \le k\}$,
3. $\{\alpha_i$ with multiplicity $n-2k : 1 \le i \le k\} \cup \{0$ with multiplicity $(n-2k)k\}$,
4. $\{0$ with multiplicity $(n-2k)^2\}$.

Note that the condition $\|\Phi(E,F)\| \le \frac{\pi}{4}$ implies $\alpha_i \le \frac{\pi}{4}$ for all i, so $\min(\alpha_i+\alpha_j, \pi-\alpha_i-\alpha_j) = \alpha_i+\alpha_j$.

Since

$$\alpha_i + \alpha_j + |\alpha_i - \alpha_j| = 2\max(\alpha_i, \alpha_j),$$

it follows that

$$(\alpha_i, \alpha_i) \prec_w (\min(\alpha_i + \alpha_j, \pi - \alpha_i - \alpha_j), |\alpha_i - \alpha_j|)$$

for all $1 \leq i, j \leq k$. Combining these k^2 weak majorizations in the manner of Proposition 1.3.9 shows that the union of the first two sets of angles of $\Phi_0(E, F)$ is weakly majorized by the union of the first two sets of angles of $\Theta(\mathcal{E}, \mathcal{F})$. Since the third set of angles of $\Phi_0(E, F)$ is weakly majorized by the third set of angles of $\Theta(\mathcal{E}, \mathcal{F})$, and the fourth sets of angles are identical, another application of Proposition 1.3.9 yields the latter half of the proposition. □

Remark 4.4.4. The condition $\|\Phi(E, F)\| \leq \frac{\pi}{4}$ is necessary and cannot be eliminated by pairing the projections E_i and F_i more efficiently. For example, consider the case where

$$P = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \text{ and } Q = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Here $\Phi_0(E, F) = (\frac{\pi}{2}, \frac{\pi}{2}, \frac{\pi}{2}, 0, 0)$ whereas $\Theta(\mathcal{E}, \mathcal{F}) = (\frac{\pi}{2}, \frac{\pi}{2}, 0, 0, 0)$, so the conclusion of the proposition fails in this case where there is only one possible pairing.

That the constant $\frac{\pi}{4}$ is the best possible can be seen in the simple example where

$$P = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \text{ and } Q = \begin{pmatrix} \cos^2\alpha & \sin\alpha\cos\alpha \\ \sin\alpha\cos\alpha & \cos^2\alpha \end{pmatrix}$$

Here $\Phi(E, F) = (\alpha, \alpha)$ while $\Theta(\mathcal{E}, \mathcal{F}) = (\min(2\alpha, \pi - 2\alpha), 0)$; thus if $\alpha > \frac{\pi}{4}$, $\Phi(E, F) \not\prec_w \Theta(\mathcal{E}, \mathcal{F})$. This example also shows that we do not have $\Phi_0(E, F) \leq \Theta(\mathcal{E}, \mathcal{F})$.

The preceding proposition shows that if $\Theta(P, Q)$ is small, then so is $\Theta(\mathcal{E}, \mathcal{F})$. If $\Theta(\mathcal{E}, \mathcal{F})$ is small, it is too much to ask that $\Theta(P, Q)$ be small; however, a reasonable request is that one of $\Theta(P, Q)$ or $\Theta(P, Q^\perp)$ be small.

Proposition 4.4.5. *Let $L = \|\Theta(\mathcal{E}, \mathcal{F})\|$ and $M = \min(\|\Theta(P, Q)\|, \|\Theta(P, Q^\perp)\|)$. (Here $\|\cdot\|$ is the bound norm.) Then $M \leq L$; if $L < \frac{\pi}{3}$, we in fact have $M = L/2$.*

Before proving this proposition we remark that the minimum over the choice of pairing P with Q or $Q^\perp$ only arises when rank $P = \frac{n}{2}$.

Proof. We write $\theta_1 \geq \cdots \geq \theta_k$ for the angles between P and Q. We have either $\theta_1 + \theta_k \leq \frac{\pi}{2}$ or $\theta_1 + \theta_k > \frac{\pi}{2}$. In the former case,

$$\theta_i \leq \theta_i + \theta_k \leq \theta_1 + \theta_k \in \Theta(\mathcal{E}, \mathcal{F})$$

for all i. In the latter case,

$$\frac{\pi}{2} - \theta_i \leq \frac{\pi}{2} - \theta_i + \frac{\pi}{2} - \theta_1 \leq \pi - \theta_k - \theta_1 \in \Theta(\mathcal{E}, \mathcal{F})$$

for all i. Thus we have either $\|\Theta(P,Q)\| \leq \|\Theta(\mathcal{E},\mathcal{F})\|$ or $\|\Theta(P,Q^\perp)\| \leq \|\Theta(\mathcal{E},\mathcal{F})\|$, so $M \leq L$ as claimed.

Now suppose $L < \frac{\pi}{3}$, so each angle in $\Theta(\mathcal{E},\mathcal{F})$ is less than $\frac{\pi}{3}$. By Proposition 4.4.1, it follows that for each i, either $2\theta_i \leq L$ or $2\theta_i \geq \pi - L > \frac{2\pi}{3}$. Suppose there are two different indices i, j for which $\theta_i \leq \frac{L}{2}$ and $\theta_j > \frac{\pi}{3}$. Then

$$L < \frac{\pi}{3} < \theta_j \leq \theta_i + \theta_j \leq \frac{L}{2} + \frac{\pi}{2} < \frac{2\pi}{3} < \pi - L.$$

Thus $\min(\theta_i + \theta_j, \pi - \theta_i - \theta_j) > L$ which contradicts $\|\Theta(\mathcal{E},\mathcal{F})\| = L$. Therefore we must have $\theta_i \leq L/2$ for all i or $\theta_i \geq \frac{\pi}{2} - \frac{L}{2}$ (that is, $\frac{\pi}{2} - \theta_i \leq \frac{L}{2}$) for all i, and so $M \leq \frac{L}{2} \leq \frac{\pi}{6}$.

Finally, wolog suppose $M = \|\Theta(P,Q)\|$, so $\theta_i \leq \frac{\pi}{4}$ for all i. It follows that $\|\Theta(\mathcal{E},\mathcal{F})\| = \max_i 2\theta_i = 2M$ as required. □

Remark 4.4.6. Note that $L = \frac{\pi}{3}$ does not imply $M \leq \frac{L}{2}$; consider the example where $\Theta(P,Q) = \{\frac{\pi}{3}, 0\}$.

4.5 General Frames

We now turn our attention to the general situation of two isomorphic ordered frames $E = (E_1, \ldots, E_r)$ and $F = (F_1, \ldots, F_r)$, where $\operatorname{rank} E_i = \operatorname{rank} F_i = n_i$. Let $\mathcal{E}$ and $\mathcal{F}$ denote the unordered frames corresponding to E and F respectively. We begin by introducing an operator $\mathcal{S}$ which will be useful in proving some of the subsequent propositions.

Suppose U is a unitary which intertwines $\mathcal{E}$ and $\mathcal{F}$, so there is a permutation $\sigma \in S_r$ such that $UE_i = F_{\sigma(i)}U$ for each $1 \leq i \leq r$. We define a map $\mathcal{S} : \mathcal{E} \to \mathcal{E}$ by $\mathcal{S}(A) = U^*(\mathcal{F}A)U$. Note that

$$U^*(\mathcal{F}A)U = U^*(\sum_{i=1}^{r} F_{\sigma(i)}AF_{\sigma(i)})U = \sum_{i=1}^{r} E_iU^*AUE_i = \mathcal{E}(U^*AU),$$

so $\phi_{U^*} \circ \mathcal{F} = \mathcal{E} \circ \phi_{U^*}$. Thus $\mathcal{S} = \phi_{U^*} \circ \mathcal{F}|_{\operatorname{Ran}\mathcal{E}} = \mathcal{E} \circ \phi_{U^*}|_{\operatorname{Ran}\mathcal{E}}$. Of course this map $\mathcal{S}$ depends on the choice of the unitary U; if there is a possible ambiguity as to what this choice of unitary is, we will write $\mathcal{S}_U$ instead.

Since we can write $\mathcal{S} = \phi_{U^*}\mathcal{F}\mathcal{E}|_{\mathrm{Ran}\,\mathcal{E}}$, we see that $\mathcal{S}^*\mathcal{S} = \mathcal{E}\mathcal{F}\mathcal{E}|_{\mathrm{Ran}\,\mathcal{E}}$, so the singular values of $\mathcal{S}$ are precisely $\cos\Theta(\mathcal{E},\mathcal{F})$. Moreover, $\mathcal{S}$ is a doubly stochastic map (positivity-preserving, unital, and trace-preserving) on $\mathcal{E}$, so $\mathcal{S}A \prec A$ for any hermitian $A \in \mathcal{E}$.

We shall find it convenient to utilize the block structure of the subalgebra $\mathcal{E}$. To this end, we will write U in block form with respect to the direct sum decomposition $\mathcal{H} = E_1\mathcal{H} \oplus \cdots \oplus E_r\mathcal{H}$ as

$$U = \begin{pmatrix} U_{11} & \dots & U_{1r} \\ \vdots & \ddots & \vdots \\ U_{r1} & \dots & U_{rr} \end{pmatrix},$$

where $U_{ij} = \iota_i^* U \iota_j$ and $\iota_j : E_j\mathcal{H} \to \mathcal{H}$ is the inclusion map. Since U is unitary, we have $U^*U = I$ and $UU^* = I$; using block notation, it follows that

$$\begin{aligned} I|_{E_i\mathcal{H}} &= \sum_{j=1}^{r} (U^*)_{ij} U_{ji} = \sum_{j=1}^{r} U_{ji}^* U_{ji}, \quad \text{and} \\ I|_{E_i\mathcal{H}} &= \sum_{j=1}^{r} U_{ij} (U^*)_{ji} = \sum_{j=1}^{r} U_{ij} U_{ij}^*, \end{aligned} \tag{4.5}$$

for all $1 \le i \le r$.

Let $A \in \mathrm{Ran}\,\mathcal{E}$, so A is block diagonal and we may write

$$A = \begin{pmatrix} A_1 & & 0 \\ & \ddots & \\ 0 & & A_r \end{pmatrix},$$

where A_i is an operator on $\mathrm{Ran}\,E_i$.

Since $\mathcal{S}A = \mathcal{E}(U^*AU)$ and $\mathcal{E}B$ is just the block diagonal of B, it follows that

$$\mathcal{S}\begin{pmatrix} A_1 & & 0 \\ & \ddots & \\ 0 & & A_r \end{pmatrix} = \begin{pmatrix} \sum_{k=1}^{r} U_{k1}^* A_k U_{k1} & & 0 \\ & \ddots & \\ 0 & & \sum_{k=1}^{r} U_{kr}^* A_k U_{kr} \end{pmatrix}.$$

We can also write $\mathcal{S}$ in a block matrix form with respect to the decomposition $\mathcal{E} = M_{n_1} \oplus \cdots \oplus M_{n_r}$, so that

$$\begin{pmatrix} \mathcal{S}_{11} & \mathcal{S}_{12} & \dots & \mathcal{S}_{1r} \\ \mathcal{S}_{21} & \mathcal{S}_{22} & & \mathcal{S}_{1r} \\ \vdots & & \ddots & \vdots \\ \mathcal{S}_{r1} & \mathcal{S}_{r2} & \dots & \mathcal{S}_{rr} \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \\ \vdots \\ A_r \end{pmatrix} = \begin{pmatrix} \sum_{j=1}^{r} \mathcal{S}_{1j} A_j \\ \sum_{j=1}^{r} \mathcal{S}_{2j} A_j \\ \vdots \\ \sum_{j=1}^{r} \mathcal{S}_{rj} A_j \end{pmatrix}$$

where $\mathcal{S}_{ij}A_j = U_{ji}^*A_jU_{ji}$ for $A_j \in M_{n_j}$. Clearly $(\mathcal{S}^*)_{ij} = \mathcal{S}_{ji}^*$. Note also that in the case where $\mathcal{E}$ is a minimal frame, $\mathcal{S}$ is just the orthostochastic matrix $os(U^*)$.

Our first proposition partly generalizes the first inequality in Prop. 4.4.3.

Proposition 4.5.1. $\Theta_k^{\uparrow}(\mathcal{E},\mathcal{F}) \leq 2\Phi_k^{\uparrow}(E,F)$ *for each* $k = 1,\ldots,n$.

Proof. Let U be a balanced transformation intertwining E and F, that is, $UE_i = F_iU$ and $E_iUE_i \geq 0$ for each i. In this case, the eigenvalues of $B = \sum_{i=1}^r E_iUE_i$ are given by $\cos\Phi$. Let $\{R_k : 1 \leq k \leq n\}$ be a set of orthogonal rank one spectral projections for B, where R_k corresponds to the eigenvalue $(\cos\Phi)_k^{\downarrow}$. Thus

$$R_kUR_k = (\cos\Phi)_k^{\downarrow}R_k. \tag{4.6}$$

Let $\iota_k : \mathrm{Span}\{R_i : 1 \leq i \leq k\} \to \mathrm{Ran}\,\mathcal{E}$ be the inclusion map; we will write $\mathcal{S}_k = \iota_k^*\mathcal{S}\iota_k$ for the compression of $\mathcal{S}$ to the subspace of $\mathrm{Ran}\,\mathcal{E}$ spanned by the orthonormal basis $\{R_i : 1 \leq i \leq k\}$. With respect to this basis, the (i,j)-entry of $\mathcal{S}_k$ is equal to

$$\begin{aligned}
\langle \mathcal{S}_kR_j, R_i\rangle &= \langle \mathcal{S}\iota_kR_j, \iota_kR_i\rangle \\
&= \langle \mathcal{S}R_j, R_i\rangle \\
&= \langle \mathcal{E}(U^*R_jU), R_i\rangle \\
&= \langle U^*R_jU, \mathcal{E}R_i\rangle \\
&= \mathrm{Tr}\,R_iU^*R_jU \\
&= \mathrm{Tr}\,R_iU^*R_jR_jUR_i \\
&= \mathrm{Tr}(R_jUR_i)^*(R_jUR_i)
\end{aligned}$$

which is non-negative. In particular, if $i = j$, (4.6) implies

$$\langle \mathcal{S}_kR_i, R_i\rangle = (\cos^2\Phi)_i^{\downarrow}. \tag{4.7}$$

Also note that $\mathcal{S}_k$ is symmetric, and that summing the entries of the jth column of $\mathcal{S}_k$ gives

$$\begin{aligned}
\sum_{i=1}^{k}\langle \mathcal{S}_kR_j, R_i\rangle &= \sum_{i=1}^{k}\mathrm{Tr}\,R_i\mathcal{S}R_j \\
&\leq \sum_{i=1}^{n}\mathrm{Tr}\,R_i\mathcal{S}R_j \\
&= \mathrm{Tr}\,\mathcal{S}R_j \\
&= \mathrm{Tr}\,R_j = 1.
\end{aligned} \tag{4.8}$$

Recall the Gershgorin Disk Theorem [4, Problem VIII.6.3] says that for a $k \times k$ matrix B,

$$\lambda(B) \subset \cup_{j=1}^{k}\{z : |z - b_{jj}| \leq \sum_{i \neq j} |b_{ij}|\}.$$

In particular, if B is self-adjoint, it follows that the smallest eigenvalue $\lambda_k(B)$ of B is greater than $\min_{j=1}^{k}(b_{jj} - \sum_{i \neq j} |b_{ij}|)$. With this in mind, we prove the proposition:

$$\begin{aligned}
(\cos\Theta)_k^{\downarrow} &= s_k^{\downarrow}(\mathcal{S}) \geq \lambda_k^{\downarrow}(\mathrm{Re}\mathcal{S}) && [4, III.5.1] \\
&\geq \lambda_k^{\downarrow}(\iota_k^*(\mathrm{Re}\mathcal{S})\iota_k) && [4, III.1.5] \\
&= \lambda_k^{\downarrow}(\mathrm{Re}\mathcal{S}_k) \\
&= \lambda_k^{\downarrow}(\mathcal{S}_k) && \text{since } \mathcal{S}_k \text{ is self-adjoint} \\
&\geq \langle \mathcal{S}_k R_k, R_k\rangle - \sum_{i=1}^{k-1} \langle \mathcal{S}_k R_k, R_i\rangle && \text{by Gershgorin Disk Theorem} \\
&\geq (\cos^2\Phi)_k^{\downarrow} - (1 - (\cos^2\Phi)_k^{\downarrow}) && \text{by (4.7) and (4.8)} \\
&= (\cos 2\Phi)_k^{\downarrow}.
\end{aligned}$$

Hence $(\cos\Theta_k)^{\downarrow} \geq (\cos 2\Phi)_k^{\downarrow}$, and so $\Theta_k^{\uparrow} \leq 2\Phi_k^{\uparrow}$ for each $k = 1, \ldots, n$, as desired. □

Remark 4.5.2. If $\mathcal{E}$ and $\mathcal{F}$ are minimal frames, then both Θ and Φ consist of n angles, so we have $\Theta_k^{\downarrow}(\mathcal{E}, \mathcal{F}) \leq 2\Phi_k^{\downarrow}(E, F)$ for all k; however, this does not hold in general. (Consider the example where $n = 4$ and $\mathcal{E}$,$\mathcal{F}$ are 2-frames with $\Phi(E, F) = (\alpha, 0)$ and $\alpha > 0$).

Proposition 4.5.3. $\|\Theta(\mathcal{E}, \mathcal{F})\|_1 \leq \|\Phi_+(E, F)\|_1$

Proof. As in Proposition 4.5.1, let U be a balanced transformation intertwining E and F; thus, using block matrix form, $U_{ii} \geq 0$ and $\mathcal{S}_{ii}A = U_{ii}AU_{ii}$. If we denote the block diagonal of $\mathcal{S}$ by $\mathcal{D} = \mathcal{S}_{11} \oplus \cdots \oplus \mathcal{S}_{rr}$, then $\mathcal{D} \geq 0$ and, since the block diagonal of $\mathcal{S}$ and $\mathrm{Re}\,\mathcal{S}$ coincide,

$$\lambda(\mathcal{D}) \prec \lambda(\mathrm{Re}\,\mathcal{S}) \leq s(\mathcal{S}) = \cos\Theta.$$

Since the eigenvalues of $\mathcal{D}$ are given by

$$\{\cos\phi_{ij}\cos\phi_{ik} : 1 \leq i \leq r, 1 \leq j, k \leq n_i\},$$

and since $\cos(\phi_{ij}+\phi_{ik}) \leq \cos\phi_{ij} + \cos\phi_{ik}$, it follows that

$$\{\cos(\phi_{ij}+\phi_{ik})\} \prec_w \cos\Theta.$$

Applying Theorem 1.3.8 to the convex increasing function $-\arccos x$ gives

$$\{-(\phi_{ij}+\phi_{ik})\} \prec_w -\Theta,$$

so in particular $-\operatorname{Tr}\Phi_+ \leq -\operatorname{Tr}\Theta$, as required. □

We now attempt to generalize the second inequality in Prop. 4.4.3.

Note that, since $\arcsin x$ is convex increasing on $[0,1]$ and $\sin^2 x$ is convex increasing on $[0,\frac{\pi}{4}]$, Theorem 1.3.8 implies that

$$\sin x \prec_w \sin y \Rightarrow x \prec_w y \Rightarrow \sin^2 x \prec_w \sin^2 y,$$

provided the coordinates of x, y lie in $[0,\frac{\pi}{4}]$. Ideally, we would like to show that $\sin\Phi_0(E,F) \prec_w \sin\Theta(\mathcal{E},\mathcal{F})$. This does not occur in general, however, regardless of how we bound $\Phi_0(E,F)$; consider the simple case where $n = r = 2$.

Thus, a first step towards showing $\Phi_0(E,F) \prec_w \Theta(\mathcal{E},\mathcal{F})$ would be to show that $\sin^2\Phi_0(E,F) \prec_w \sin^2\Theta(\mathcal{E},\mathcal{F})$ if $\|\Phi_0(E,F)\| \leq \frac{\pi}{4}$. The next proposition is a partial result in that direction.

Proposition 4.5.4. *If $\mathcal{E}$ and $\mathcal{F}$ are minimal frames then*

$$2\sin^2\Phi_0(E,F)\cos^2\Phi_0(E,F) \prec_w \sin^2\Theta(\mathcal{E},\mathcal{F}).$$

Before beginning the proof, we introduce a short lemma.

Lemma 4.5.5. *If $a = (a_1,\ldots,a_r)$ and $b = (b_1,\ldots,b_r)$ are probability vectors (that is, all coordinates are non-negative and sum to 1), then*

$$1 - a\cdot b \geq a_i(1-b_i) + b_i(1-a_i) \tag{4.9}$$

for all $1 \leq i \leq r$.

Proof of Lemma. We have

$$a\cdot b = \sum_{j=1}^{r} a_j b_j \leq a_i b_i + (\sum_{j\neq i} a_j)(\sum_{j\neq i} b_j) = a_i b_i + (1-a_i)(1-b_i) \tag{4.10}$$

for any index i. Thus

$$1 - a\cdot b \geq a_i + b_i - 2a_i b_i = a_i(1-b_i) + b_i(1-a_i)$$

for all i, as required. □

Proof of Proposition. Let U be a balanced transformation intertwining E and F, so $UE_i = F_iU$ and $E_iUE_i \geq 0$ for each i. In particular, we may assume that U_{ii} is diagonal for each i and write

$$U_{ii} = \begin{pmatrix} \cos\phi_{i1} & & 0 \\ & \ddots & \\ 0 & & \cos\phi_{in_i} \end{pmatrix}.$$

Writing $\operatorname{Ran}\mathcal{E} = M_{n_1}\oplus\cdots\oplus M_{n_r}$, we let $\mathcal{T}_i : M_{n_i} \to M_{n_i}$ denote the compression of $\mathcal{E}\mathcal{F}\mathcal{E} = \mathcal{S}^*\mathcal{S}$ to M_{n_i}; thus if $A \in M_{n_i}$, $\mathcal{T}_i(A) = \sum_{j=1}^r U_{ij}U_{ij}^*AU_{ij}U_{ij}^*$. Let $C_{ij} = U_{ij}U_{ij}^*$. We compute the diagonal entries of $\mathcal{T}_i$ with respect to the standard orthonormal basis $\{e_ke_l^*\}$ on M_{n_i}:

$$\langle \mathcal{T}_i(e_ke_l^*), e_ke_l^*\rangle = \operatorname{Tr} e_le_k^* \sum_{j=1}^r C_{ij}e_ke_l^*C_{ij} = \sum_{j=1}^r (C_{ij})_{kk}(C_{ij})_{ll}. \tag{4.11}$$

But since $C_{ij} \geq 0$ and $\sum_{j=1}^r C_{ij} = I$ by (4.5), $((C_{i1})_{kk}, \dots, (C_{ir})_{kk})$ is a probability vector for each i and k. It follows from (4.11) and (4.9) that

$$\begin{aligned}\langle (id - \mathcal{T}_i)(e_ke_l^*), e_ke_l^*\rangle &\geq (C_{ii})_{kk}(1-(C_{ii})_{ll}) + (C_{ii})_{ll}(1-(C_{ii})_{kk}) \\ &= \cos^2\phi_{ik}\sin^2\phi_{il} + \cos^2\phi_{il}\sin^2\phi_{ik}\end{aligned}$$

for any i, k, l.

Thus if $\mathcal{P}_i$ is the projection onto M_{n_i} we have

$$\begin{aligned}\cup_{i,k,l}\cos^2\phi_{ik}\sin^2\phi_{il} + \cos^2\phi_{il}\sin^2\phi_{ik} &\leq \cup_{i=1}^r \operatorname{diag}(id|_{M_{n_i}} - \mathcal{T}_i)) \\ &\prec \cup_{i=1}^r \lambda(id - \mathcal{T}_i) \\ &= \lambda(\sum_{i=1}^r \mathcal{P}_i\mathcal{E}\mathcal{F}^\perp\mathcal{E}\mathcal{P}_i) \\ &\prec \sigma(\mathcal{E}\mathcal{F}^\perp\mathcal{E}) \\ &= \sin^2\Theta(\mathcal{E},\mathcal{F})\end{aligned}$$

But if $\mathcal{E}, \mathcal{F}$ are minimal then the left hand side is just $2\sin^2\Phi_0(E,F)\cos^2\Phi_0(E,F)$, and the proposition follows. □

Remark 4.5.6. If $\|\Phi(E,F)\| \leq \frac{\pi}{4}$ then we have

$$\{\frac{1}{2}(\sin^2\phi_{ik} + \sin^2\phi_{il}) : 1 \leq i \leq r; 1 \leq k, l \leq n_i\} \prec_w \sin^2\Theta(\mathcal{E},\mathcal{F})$$

where E and F need not be minimal. In particular, this shows that $\|\Phi(E,F)\| \leq \|\Theta(\mathcal{E},\mathcal{F})\|$. If E and F are minimal we have $\sin^2\Phi_0(E,F) \prec_w \sin^2\Theta(\mathcal{E},\mathcal{F})$.

The 2-frame example where $\Phi(E,F) = (\alpha, 0, \ldots, 0)$, rank E = rank $E^\perp$, and α is sufficiently small shows we do not have $2\sin^2\Phi_0(E,F)\cos^2\Phi_0(E,F) \prec_w \sin^2\Theta(\mathcal{E},\mathcal{F})$ in general.

The next result generalizes Proposition 4.4.5; it says that if $\|\Theta(\mathcal{E},\mathcal{F})\|$ is small, then there is a way to pair the projections of $\mathcal{E}$ and $\mathcal{F}$ so that $\|\Phi(E,F)\|$ is small.

Proposition 4.5.7. *Let $\mathcal{E} = \{E_1,\ldots,E_r\}, \mathcal{F} = \{F_1,\ldots,F_r\}$ be two isomorphic frames. Suppose $\|\Theta(\mathcal{E},\mathcal{F})\| = \alpha < \frac{\pi}{4}$. Then there exists a unique permutation σ such that all angles ϕ_{ij} between the ordered frames $(E_1,\ldots,E_r)$ and $(F_{\sigma(1)},\ldots,F_{\sigma(r)})$ are less than α.*

Proof. The case $\alpha = 0$ is trivial so assume $\alpha > 0$. The hypothesis implies that for all angles $\theta_j \in \Theta(\mathcal{E},\mathcal{F})$, $\cos^2\theta_j \geq \cos^2\alpha$, so $\mathcal{EFE} \geq \cos^2\alpha\,\mathcal{E}$. In particular, for any index $i = 1,\ldots,r$ the compression $\mathcal{T}_i$ of $\mathcal{EFE}$ to M_{n_i} defined in Prop. 4.5.4 must satisfy

$$\langle \mathcal{T}_i A, A\rangle \geq \cos^2\alpha \tag{4.12}$$

for any $A \in M_{n_i}$ with norm $\|A\|_2 = 1$.

Fix a unit vector $x \in \operatorname{Ran} E_i$. Letting $A = xx^*$ in (4.12) gives

$$\begin{aligned}\cos^2\alpha &\leq \operatorname{Tr} xx^*\mathcal{T}_i(xx^*)\\ &= \operatorname{Tr} xx^*\sum_{j=1}^r C_{ij}xx^*C_{ij}\\ &= \sum_{j=1}^r (x^*C_{ij}x)^2,\end{aligned}$$

where, as in Prop. 4.5.4, $C_{ij} = U_{ij}U_{ij}^*$.

Suppose, by way of contradiction, that $x^*C_{ij}x \leq \cos^2\alpha$ for all j. It follows that

$$(x^*C_{i1}x,\ldots,x^*C_{ir}x) \prec (1-\cos^2\alpha, \cos^2\alpha, 0,\ldots,0),$$

so, by applying Theorem 1.3.8 with the convex function $f(t) = t^2$,

$$\sum_{j=1}^r (x^*C_{ij}x)^2 \leq (\cos^2\alpha)^2 + (1-\cos^2\alpha)^2.$$

This implies

$$\begin{aligned}\cos^2\alpha &\le (\cos^2\alpha)^2 + (1-\cos^2\alpha)^2 \\ &= \cos^2\alpha + \sin^2\alpha(\sin^2\alpha - \cos^2\alpha) \\ &< \cos^2\alpha \qquad\qquad \text{since } 0<\alpha<\frac{\pi}{4},\end{aligned}$$

which is a contradiction. Thus there must be some index j for which $x^*C_{ij}x > \cos^2\alpha$. Wolog assume $j = 1$.

Let y be a unit vector in $\operatorname{Ran} E_i$ and write $\lambda = x^*C_{i1}x$ and $\mu = y^*C_{i1}y$. Letting $A = xy^*$ in (4.12) implies

$$\begin{aligned}\cos^2\alpha &\le \operatorname{Tr} yx^*T_i(xy^*) \\ &= \operatorname{Tr} yx^*\sum_{j=1}^{r} C_{ij}xy^*C_{ij} \\ &= \sum_{j=1}^{r}(x^*C_{ij}x)(y^*C_{ij}y) \\ &\le \lambda\mu + (1-\lambda)(1-\mu),\end{aligned}$$

where we have used (4.10) applied to the probability vectors $(x^*C_{i1}x,\ldots,x^*C_{ir}x)$, $(y^*C_{i1}y,\ldots,y^*C_{ir}y)$ for the last inequality. The last quantity is a convex combination of μ and $1-\mu$; since $\lambda > \frac{1}{2}$, it must lie between μ and $\frac{1}{2}$. Since $\cos^2\alpha > \frac{1}{2}$, the inequality can only occur if $\mu \ge \cos^2\alpha$. Since y was arbitrary, we conclude that $C_{i1} \ge \cos^2\alpha\, E_i$.

Thus we have shown that for each index i there exists an index j such that $C_{ij} \ge \cos^2\alpha\, E_i > \frac{1}{2}E_i$. Since $\sum_{j=1}^{r} C_{ij} = I$, this index j is unique, and so we can write $j = \sigma(i)$ for some permutation $\sigma \in S_r$.

Since $U_{i\sigma(i)}U^*_{i\sigma(i)} = C_{i\sigma(i)} \ge \cos^2\alpha\, E_i$, $C_{i\sigma(i)}$ is invertible and so $U^*_{i\sigma(i)} : \operatorname{Ran} E_i \to \operatorname{Ran} E_{\sigma(i)}$ has zero kernel, so rank $E_i \le$ rank $E_{\sigma(i)}$. Thus rank E_k is constant for all indices k belonging to the same cycle of σ, that is, σ permutes blocks of the same size.

Thus we can pair E_i with $F_{\sigma(i)}$ and the cosines of the angles between these two projections are given by the singular values of $U_{i\sigma(i)}$, all of which are greater than $\cos\alpha$. But the arccos of these singular values are just the angles between the ordered frames $(E_1,\ldots,E_r)$ and $(F_1,\ldots,F_r)$, proving the proposition. □

4.6 Summary

For the special case of 2-frames, we obtained our strongest result:

$$\Phi_0(E,F) \prec_w \Theta(\mathcal{E},\mathcal{F}) \le \Phi_+(E,F) \prec 2\Phi_0(E,F)$$

where we require $\|\Phi(E,F)\| \le \frac{\pi}{4}$ for the weak majorization. We conjecture that this holds in general; here we summarize the results we have thus far.

For minimal frames, note that $\Phi(E,F) = \Phi_0(E,F) = \frac{1}{2}\Phi_+(E,F)$. Our best results here are

$$2\sin^2\Phi\cos^2\Phi \prec_w \sin^2\Theta \le \Phi_+ \prec 2\Phi;$$

note that for $\|\Phi\| \le \frac{\pi}{4}$ we have

$$\sin^2\Phi \prec_w \sin^2\Theta.$$

For frames in general, much less is known. We do have

1. $\|\Phi_0\| \le \|\Theta\|$ (if $\|\Phi_0\| \le \frac{\pi}{4}$). This follows from Remark 4.5.6.

2. $\|\Theta\| \le \|\Phi_+\| = \|2\Phi_0\|$. This is obtained by almost the exact same argument as in Proposition 4.5.1.

3. $\operatorname{Tr}\Theta \le \operatorname{Tr}\Phi_+ = \operatorname{Tr}2\Phi_0$. This is just Proposition 4.5.3.

We also have a negative result: we do not have $\sin\Phi_0 \prec_w \sin\Theta$ in general, even for 2-frames or minimal frames, regardless of any bounds we might impose on $\|\Phi_0\|$ (see the simple case where $n = 2, r = 2$).

Chapter 5

Antipodal Frames

We return to the idea that if A lies in the range of $\mathcal{E}$ and if $\mathcal{E}$ and $\mathcal{F}$ are close, one would expect that $\mathcal{F}A$ is only slightly more messed up than A. Conversely, if $\mathcal{G}\mathcal{E}A \prec \mathcal{F}\mathcal{E}A$ for all hermitian A then surely $\mathcal{G}$ is farther from $\mathcal{E}$ than $\mathcal{F}$ is. From this viewpoint, a frame $\mathcal{F}$ should be maximally distant from $\mathcal{E}$ precisely if $\mathcal{F}\mathcal{E}A = (\frac{1}{n}\operatorname{Tr} A)I$ for any A. We shall pursue this idea further in this chapter, asking which pairs of frames possess this property, and how many are there. First we introduce some notation.

Definition 5.0.1. We say two frames $\mathcal{E}$ and $\mathcal{F}$ are *antipodal* if $\mathcal{E}\mathcal{F}A = (\frac{1}{n}\operatorname{Tr} A)I$ for all $A \in M_n$.

Note that, since the map $\Psi(A) = (\frac{1}{n}\operatorname{Tr} A)I$ is a projection in $\mathcal{B}(M_n)$, $\mathcal{E}\mathcal{F} = \Psi$ if and only if $\mathcal{F}\mathcal{E} = \Psi$. Thus the definition is symmetric in $\mathcal{E}$ and $\mathcal{F}$. The definition also allows the possibility that $\mathcal{E}$ and $\mathcal{F}$ are non-isomorphic; the following lemma shows that this never occurs.

Lemma 5.0.2. *Let $\mathcal{E} = \{E_1, \ldots, E_r\}$ and $\mathcal{F} = \{F_1, \ldots, F_s\}$ be two (not necessarily isomorphic) frames. Then $\mathcal{E}$ and $\mathcal{F}$ are antipodal if and only if both $\mathcal{E}$ and $\mathcal{F}$ are minimal frames and $\operatorname{Tr} E_iF_j = \frac{1}{n}$ for all i, j.*

Proof. For the 'if' part, write $E_i = e_ie_i^*, F_j = f_jf_j^*$ for some orthonormal bases $\{e_i\}, \{f_j\}$ of $\mathbb{C}^n$. Then since $\operatorname{Tr} E_iF_j = e_i^*f_jf_j^*e_i$, it follows that

$$\begin{aligned}\mathcal{F}\mathcal{E}A &= \sum_{i,j=1}^{n} f_j f_j^* e_i e_i^* A e_i e_i^* f_j f_j^* \\ &= \sum_{i,j=1}^{n} (\operatorname{Tr} E_i F_j)(e_i^* A e_i) F_j \\ &= (\frac{1}{n} \operatorname{Tr} A) I\end{aligned}$$

for any matrix A, as required.

For the 'only if' part, let P be a rank one projection in the range of $\mathcal{E}$, so

$$\sum_{j=1}^{s} F_j P F_j = \mathcal{F}P = \mathcal{F}\mathcal{E}P = \frac{1}{n} I = \sum_{j=1}^{s} \frac{1}{n} F_j.$$

This implies that

$$F_j P F_j = \frac{1}{n} F_j \tag{5.1}$$

for each j. Since the left hand side has rank at most one, it follows that rank $F_j = 1$ for each j. Due to the symmetry in the definition of antipodal frames, we can reverse the roles of $\mathcal{E}$ and $\mathcal{F}$ to conclude rank $E_i = 1$ for each i. Thus $\mathcal{E}$ and $\mathcal{F}$ are both minimal frames. Finally, setting $P = E_i$ in (5.1) and taking the trace implies $\operatorname{Tr} E_i F_j = \frac{1}{n}$ for each i, j, as required. □

From the notation used, one might wonder if two antipodal frames really are maximally far apart with respect to some natural metric. The following proposition shows that this is indeed the case.

Proposition 5.0.3. *Let $1 \leq p < \infty$ and define the distance between two minimal frames $\mathcal{E}, \mathcal{F}$ by $\|\mathcal{E} - \mathcal{F}\|_p$ (here $\mathcal{E}$ and $\mathcal{F}$ are viewed as operators on the Hilbert-Schmidt space M_n). Then $\mathcal{E}$ and $\mathcal{F}$ are antipodal if and only if $\|\mathcal{E} - \mathcal{F}\|_p$ is the maximum distance between any two minimal frames.*

Proof. Let $\mathcal{E}$ and $\mathcal{F}$ be two minimal frames. Since $\mathcal{E}$ and $\mathcal{F}$ are projections on M_n of the same rank, [4, p.201] shows that

$$\|\mathcal{E} - \mathcal{F}\| = \|\sin\Theta(\mathcal{E}, \mathcal{F}) \oplus \sin\Theta(\mathcal{E}, \mathcal{F})\|$$

for any unitarily invariant norm. Since I lies in the range of both $\mathcal{E}$ and $\mathcal{F}$, at least one of the angles in $\Theta(\mathcal{E},\mathcal{F})$ is zero; hence $\|\mathcal{E}-\mathcal{F}\|_p$ is maximized iff all the other angles in $\Theta(\mathcal{E},\mathcal{F})$ are $\frac{\pi}{2}$. Since $\cos^2\Theta(\mathcal{E},\mathcal{F})$ consists of the eigenvalues of $\mathcal{E}\mathcal{F}\mathcal{E}$, this is equivalent to requiring that the spectrum of $\mathcal{E}\mathcal{F}\mathcal{E}$ has only one nonzero eigenvalue. Thus $\|\mathcal{E}-\mathcal{F}\|_p$ is maximized iff $\mathcal{E}\mathcal{F}\mathcal{E}$ has rank one iff $\mathcal{F}\mathcal{E}$ has rank one. Since both $\mathcal{E}$ and $\mathcal{F}$ fix I and are trace-preserving, it follows that $\|\mathcal{E}-\mathcal{F}\|_p$ is maximal iff $\mathcal{F}\mathcal{E}A = (\frac{1}{n}\operatorname{Tr}A)I$, as required. ∎

Remark 5.0.4. Note that the proof in fact shows more; if $\mathcal{E}$ and $\mathcal{F}$ are antipodal, then they are maximally distant with respect to *any* unitarily invariant norm. The converse is not true in general; two frames $\mathcal{E}$ and $\mathcal{F}$ may be maximally distant with respect to the bound norm, but not be antipodal.

To avoid any possible confusion, I shall use the term antipodal only in the sense of the above proposition; for a general metric ρ on the space of minimal frames I will speak of two frames being maximally distant with respect to ρ.

A natural question is to find all frames $\mathcal{F}$ antipodal from a given frame $\mathcal{E}$. Lemma 5.0.2 shows that for this to occur, both $\mathcal{E},\mathcal{F}$ must be minimal frames, so $\mathcal{E}=\{e_ie_i^*\}$, $\mathcal{F}=\{f_if_i^*\}$ for some orthonormal bases $\{e_i\}$, $\{f_i\}$ of $\mathbb{C}^n$. If $U=(e_1|\dots|e_n)$ and $V=(f_1|\dots|f_n)$, then $\mathcal{E},\mathcal{F}$ can be identified with the (left) cosets $[U],[V]\in U_n/H$ respectively (here H is the subgroup of U_n generated by the permutation matrices and diagonal unitaries). Since $\operatorname{Tr}E_iF_j=|f_j^*e_i|^2$, the condition $\operatorname{Tr}E_iF_j=\frac{1}{n}$ for all i,j is equivalent to the requirement that $os(Y^*X)=J_n$ for some (any) choice of representatives X of $[U]$ and Y of $[V]$; in particular,

$$[U] \text{ and } [V] \text{ are antipodal } \iff os(V^*U)=J_n \tag{5.2}$$

(recall $os(U)$ is the matrix whose (i,j)-entry is $|U_{ij}|^2$). It follows that $[U]$ and $[V]$ are antipodal if and only if $[V^*U]$ and $[I]$ are, so it suffices to find all frames antipodal from $[I]$; that is, we wish to find all unitaries U for which $os(U)=J_n$. Note that if $os(U)=J_n$ then $os(U')=J_n$ for any unitary U' in the same double coset of H as U, so we may restrict our search to those unitaries U for which all the entries in the first row and column are equal to $\frac{1}{\sqrt{n}}$.

Proposition 5.0.5. *Suppose U is unitary and $os(U)=J_n$. If $n=2,3$, or 4 then U must lie in the same double coset as*

$$\frac{1}{\sqrt{2}}\begin{pmatrix}1&1\\1&-1\end{pmatrix},\ \frac{1}{\sqrt{3}}\begin{pmatrix}1&1&1\\1&\omega&\bar{\omega}\\1&\bar{\omega}&\omega\end{pmatrix},\ \text{or } F(\alpha)=\frac{1}{2}\begin{pmatrix}1&1&1&1\\1&1&-1&-1\\1&-1&\alpha&-\alpha\\1&-1&-\alpha&\alpha\end{pmatrix}$$

respectively, where $\omega = e^{2\pi i/3}$ *and* α *is a complex number of modulus one.*

Proof. The $n = 2$ case is trivial. For the other cases, it is helpful to view complex numbers as vectors in the plane. For $n = 3$, note that a triple (a_1, a_2, a_3) of complex numbers satisfies $a_1 + a_2 + a_3 = 0$ and $|a_i| = 1$ for each i only if the triple denotes the sides of an equilateral triangle. The result follows almost immediately by noting that the rows of U are orthonormal. For $n = 4$, note that a quadruple (b_1, b_2, b_3, b_4) of complex numbers satisfies $b_1 + b_2 + b_3 + b_4 = 0$ and $|b_i| = 1$ for each i only if the quadruple denotes the sides of a rhombus, in which case one may assume wolog that $b_2 = -b_1$ and $b_4 = -b_3$. Noting that the rows of U are orthonormal and considering the various possibilities entailed by this argument gives the result for $n = 4$. □

Remark 5.0.6. Note that there is a unique double coset of unitaries with associated orthostochastic matrix J_n for $n = 2, 3$ but not for $n = 4$; in fact $F(\alpha)$ and $F(\beta)$ lie in the same double coset if and only if $\beta = \pm\alpha$ (in which case they actually lie in the same coset). This relative abundance of double cosets with associated orthostochastic matrix for $n = 4$ is representative of the situation where n is composite.

Proposition 5.0.7. *Let* F_p *denote the* $p \times p$ *finite fourier transform, so* $(F_p)_{jk} = \frac{1}{\sqrt{p}}\exp(\frac{2\pi i}{p}(j-1)(k-1))$, $1 \le j, k \le p$. *Let* $D \in M_{pq}$ *be the block matrix*

$$\begin{pmatrix} I & D_1 & \dots & D_{p-1} \\ \vdots & \vdots & & \vdots \\ I & D_1 & \dots & D_{p-1} \end{pmatrix},$$

where for each j, $D_j \in M_q$ *is a diagonal unitary with* $(1,1)$*-entry equal to one. Let* $\circ$ *denote the block Hadamard product, so if* A *and* B *are block matrices,*

$$\begin{pmatrix} A_{11} & \dots & A_{p1} \\ \vdots & \ddots & \vdots \\ A_{p1} & \dots & A_{pp} \end{pmatrix} \circ \begin{pmatrix} B_{11} & \dots & B_{p1} \\ \vdots & \ddots & \vdots \\ B_{p1} & \dots & B_{pp} \end{pmatrix} = \begin{pmatrix} A_{11}B_{11} & \dots & A_{p1}B_{p1} \\ \vdots & \ddots & \vdots \\ A_{p1}B_{p1} & \dots & A_{pp}B_{pp} \end{pmatrix}.$$

Then the $pq \times pq$ *matrix* $(F_p \otimes F_q) \circ D$ *is unitary with associated orthostochastic matrix* J_{pq}.

Proof. Let $U = (F_p \otimes F_q) \circ D$. The (i, j)-block of U is given by the $q \times q$ matrix $U_{ij} = (F_p)_{ij} F_q D_j$. The modulus of each entry in this block is $\frac{1}{\sqrt{p}}\frac{1}{\sqrt{q}}$, which shows that

$os(U) = J_{pq}$. To see that U is unitary, note that the (i,k)-block of U^*U is given by

$$\begin{aligned}\sum_{j=1}^{p}(U^*)_{ij}U_{jk} &= \sum_{j=1}^{p}(U_{ji})^*U_{jk}\\ &= \sum_{j=1}^{p}((F_p)_{ji}F_qD_i)^*(F_p)_{jk}F_qD_k\\ &= \sum_{j=1}^{p}(\overline{F_p})_{ji}(F_p)_{jk}D_i^*F_q^*F_qD_k\\ &= (F_p^*F_p)_{ik}D_i^*D_k = \delta_{ik}D_i^*D_k.\end{aligned}$$

□

Remark 5.0.8. The number of double cosets of unitaries with associated orthostochastic matrix J_n is related to the 2-transitivity of the action of U_n on antipodal pairs. (Recall that a unitary U acts on a frame $[A]$ via $U[A] = [UA]$.) Here we say that the action of U_n is *2-transitive* if, whenever $([A_1],[A_2])$ and $([B_1],[B_2])$ are antipodal pairs of frames, there exists a unitary U for which $U[A_i] = [B_i]$, $i = 1,2$.

Since $A_1^{-1}([A_1],[A_2]) = ([I],[A_1^{-1}A_2])$, U_n is 2-transitive if and only if whenever $[A]$ and $[B]$ are antipodal from $[I]$ there exists a unitary U for which $U[I] = [I]$ and $U[A] = [B]$. Since $U[I] = [I]$ iff $U \in H$, the condition $U[A] = [B]$ says that A and B lie in the same double coset. Thus U_n is 2-transitive if and only if all frames antipodal from $[I]$ lie in the same double coset. In particular, we have 2-transitivity when $n = 2$ or 3 but not when n is composite.

Beyond this, not much is known. An obvious question is what happens when n is prime. For $n = 5$, Drury [9] has recently shown numerically that the only double coset of unitaries with associated orthostochastic matrix J_5 is that containing the finite fourier transform. However, Drury [8] has also shown that for $n = 7$, there is at least one dimension worth of double cosets of unitaries which have associated orthostochastic matrix J_7. It is not clear what happens for larger primes.

5.1 Maximal Antipodal Sets

In the previous section we asked which frames are farthest apart from each other. In this section we want to obtain an idea of how 'spread out' the space of frames is; in particular, how many frames can be antipodal to each other?

Definition 5.1.1. A *maximal antipodal* set is a set of frames $\{[A_1], \dots, [A_k]\}$ satisfying:

1. $[A_i]$ and $[A_j]$ are antipodal whenever $i \neq j$.
2. Any strictly larger collection containing $\{[A_1], \dots, [A_k]\}$ does not have the above property.

Remark 5.1.2. Note that (5.2) shows that $\{[A_1], \dots, [A_k]\}$ is a set of mutually antipodal frames if and only if $\{[UA_1], \dots, [UA_k]\}$ is for any unitary U, so in searching for maximal antipodal sets one may assume wolog that $A_1 = I$ and that A_2 is one of the unitaries listed in Proposition 5.0.5.

Proposition 5.1.3. *For $n = 2$, the maximal antipodal sets are obtained by the action of U_n on sets of the form*

$$\{[I], \left[\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\right], \left[\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}\right]\}. \tag{5.3}$$

Proof. By Remark 5.1.2, it suffices to find all maximal antipodal sets containing $[I]$ and $[U]$, where

$$U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

If a frame $[V]$ is antipodal from $[I]$, Proposition 5.0.5 implies that $[V]$ is represented by hU for some $h \in H$. But both U and σU (here σ is the permutation $J - I$) represent the same coset since

$$\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Since A and $e^{i\theta}A$ represent the same coset, it follows that we may write

$$V = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ \mu & -\mu \end{pmatrix}$$

for some μ of modulus one. If $[V]$ is also antipodal from $[U]$ we must have $os(U^*V) = J_2$. That the (1,1) entry of $os(U^*V)$ equals $\frac{1}{2}$ implies that

$$\frac{1}{4}(2 + 2 \text{ Re } \mu) = \frac{1}{2} \Rightarrow \mu = \pm i.$$

Hence we can represent $[V]$ by

$$V = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix},$$

proving the proposition. □

Proposition 5.1.4. *For $n = 3$, the maximal antipodal sets are obtained by the action of U_n on sets of the form*

$$\{[I], \left[\frac{1}{\sqrt{3}}\begin{pmatrix} 1 & 1 & 1 \\ 1 & \omega & \bar{\omega} \\ 1 & \bar{\omega} & \omega \end{pmatrix}\right], \left[\frac{1}{\sqrt{3}}\begin{pmatrix} 1 & 1 & 1 \\ 1 & \omega & \bar{\omega} \\ \omega & 1 & \bar{\omega} \end{pmatrix}\right], \left[\frac{1}{\sqrt{3}}\begin{pmatrix} 1 & 1 & 1 \\ 1 & \omega & \bar{\omega} \\ \bar{\omega} & \omega & 1 \end{pmatrix}\right]\}$$

where ω is a primitive cube root of unity.

Proof. By Remark 5.1.2, it suffices to find all maximal antipodal sets containing $[I]$ and $[U]$, where

$$U = \begin{pmatrix} 1 & 1 & 1 \\ 1 & \omega & \bar{\omega} \\ 1 & \bar{\omega} & \omega \end{pmatrix}.$$

If a frame $[V]$ is antipodal from $[I]$, Proposition 5.0.5 implies that $[V]$ is represented by hU for some $h \in H$. But both U and σU represent the same coset for any permutation $\sigma \in S_3$ since we can choose $\rho \in S_3$ and a diagonal unitary d such that $\sigma U = U d \rho$. As A and $e^{i\theta}A$ represent the same coset, it follows that we may write

$$V = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 & 1 & 1 \\ \gamma & \gamma\omega & \gamma\bar{\omega} \\ \delta & \delta\bar{\omega} & \delta\omega \end{pmatrix},$$

where $|\gamma| = |\delta| = 1$. If $[V]$ is also antipodal from $[U]$ we must have $os(U^*V) = J_3$.

That the modulus of the (1,1) and (1,2) entries of $os(U^*V)$ is $\frac{1}{3}$ gives

$$|1 + \gamma + \delta| = \sqrt{3},$$
$$|1 + \omega\gamma + \bar{\omega}\delta| = \sqrt{3}.$$

Writing $x = e^{i\theta} = \gamma$ and $y = e^{i\phi} = \delta$, this translates into

$$\begin{aligned} \text{Re } x + \text{Re } y + \text{Re } x\bar{y} &= 0, \\ \text{Re } \omega x + \text{Re } \bar{\omega} y + \text{Re } \bar{\omega} x\bar{y} &= 0, \end{aligned} \tag{5.4}$$

or equivalently,

$$\cos(\theta)+\cos(\phi) = -\cos(\theta-\phi),$$
$$-\sin(\theta)+\sin(\phi) = -\sin(\theta-\phi).$$

Squaring both equations and summing implies $\cos(\theta+\phi) = -\frac{1}{2}$, so $xy=\omega$ or $\bar{\omega}$, that is, $y = e^{\pm\frac{2\pi i}{3}}\bar{x}$. But equations (5.4) say that

$$\mathrm{Re}(\bar{x}+y+x\bar{y}) = \mathrm{Re}\,\bar{\omega}(\bar{x}+y+x\bar{y}) = 0,$$

which implies that $\bar{x}+y+x\bar{y}=0$. Multiplying this equation by x and substituting for y implies that $x^3=1$. Thus $x=1,\omega,$ or $\bar{\omega}$, with the corresponding values for y given by noting $xy=\omega$ or $\bar{\omega}$. Consideration of all possible choices of x and y shows that V must lie in the same coset as one of

$$\frac{1}{\sqrt{3}}\begin{pmatrix}1 & 1 & 1\\ 1 & \omega & \bar{\omega}\\ \omega & 1 & \bar{\omega}\end{pmatrix} \text{ or } \frac{1}{\sqrt{3}}\begin{pmatrix}1 & 1 & 1\\ 1 & \omega & \bar{\omega}\\ \bar{\omega} & \omega & 1\end{pmatrix}.$$

One can verify that the two cosets represented by these two matrices are antipodal to $[I],[U]$ and to each other, and so the proposition follows. □

Proposition 5.1.5. *If $v\in\mathbb{C}^n$, let diag(v) denote the diagonal matrix whose jth diagonal entry is v_j. For n = 4, the maximal antipodal sets are obtained by the action of U_n on sets of either the form:*

$$\{[I], F[\alpha], [diag(a,a,c,-c)F(\beta)]\}$$

if $\alpha\neq\pm1$ (here a,c,β are arbitrary complex numbers of modulus one), or

$$\{[I],[F(1)],[h_1F(1)],[h_2F(1)],[h_3F(1)]\}$$

where $h_1 = diag(1,1,i,-i)$, $h_2 = diag(1,i,-i,1)$, and $h_3 = diag(1,-i,1,i)$.

Before proving this proposition two lemmas are needed.

Lemma 5.1.6. *Let a,b,c,d be complex numbers of modulus one. Then*

$$|a+b+c+d| = |a+b-c-d| = 2 \tag{5.5}$$

if and only if two of a,b,c,d are equal and the other two sum to zero.

Proof. The 'if' part is easy to verify. For the 'only if' part, note that if one regards two complex numbers x, y as vectors in the complex plane, then

$$|x+y| = |x-y| \Rightarrow x \perp y,$$

(that is, $\operatorname{Re} y^* x = 0$). Let $x = a+b, y = c+d$ to see that $a+b \perp c+d$. Applying Pythagoras gives

$$\begin{aligned} 4 &= |(a+b)+(c+d)|^2 = |a+b|^2 + |c+d|^2 \\ &\Rightarrow 0 = 2\operatorname{Re}(a\bar{b} + c\bar{d}) && \text{since } a, b, c, d \text{ have modulus 1} \\ &\Rightarrow \operatorname{Re} c\bar{d} = \operatorname{Re}(-a)\bar{b}. \end{aligned}$$

Geometrically, this says that the angle between c and d equals the angle between $-a$ and b. Let $k = -\bar{b}a$, so $kb = -a$; that is, applying k rotates b onto $-a$. It follows that either $kd = c$ or $\bar{k}d = c$.

Case 1. First consider $kd = c$. In this case

$$\begin{aligned} a+b \perp c+d &\Rightarrow a - \bar{k}a \perp c + c\bar{k} \\ &\Rightarrow 0 = \operatorname{Re} c(1+\bar{k})\bar{a}(1-k) = \operatorname{Re} c\bar{a}(-2i \operatorname{Im} k) \\ &\Rightarrow \operatorname{Im} k = 0 \text{ or } c\bar{a} = \pm 1. \end{aligned}$$

Thus either $c = \pm a$ or $k = \pm 1$, in which case $b = \pm a$. Together with (5.5) this gives the desired conclusion.

Case 2. Now consider $\bar{k}d = c$. In this case

$$\begin{aligned} a+b \perp c+d &\Rightarrow a - \bar{k}a \perp d\bar{k} + d \\ &\Rightarrow 0 = \operatorname{Re} d(1+\bar{k})\bar{a}(1-k) = \operatorname{Re} d\bar{a}(-2i \operatorname{Im} k) \\ &\Rightarrow \operatorname{Im} k = 0 \text{ or } d\bar{a} = \pm 1. \end{aligned}$$

Thus either $d = \pm a$ or $k = \pm 1$, in which case $b = \pm a$. Together with (5.5) this gives the desired conclusion.

□

Remark 5.1.7. Note that the preceding lemma asserts that $\{a, b, c, d\}$ can be grouped into two pairs of parallel vectors.

Lemma 5.1.8. *Suppose a, b, c, d satisfy the hypotheses of Lemma 5.1.6. Suppose also*

$$|a - b + \gamma c - \gamma d| = 2 \tag{5.6}$$

for some complex number γ of modulus one. Then either $a \parallel b$ (that is, $a = \pm b$) or $\gamma = \pm 1$.

Proof. Suppose $a \nparallel b$. We wish to show $\gamma = \pm 1$. Applying Lemma 5.1.6 shows that a is parallel to one of b, c, d; since the conditions are symmetric in c and d (we don't care whether we have γ or $-\gamma$), wolog assume $a \parallel c$, so $a = c$ or $a = -c$. Suppose $a = c$, so necessarily $b = -d$. Then

$$a - b + \gamma c - \gamma d = a - b + \gamma a + \gamma b = (a - b) + \gamma(a + b)$$

has norm 2. Since $(a-b)+(a+b)$ and $(a-b)-(a+b)$ both have norm 2 and since the set $\{(a-b)+e^{i\theta}(a+b) : \theta \in [0, 2\pi]\}$ can intersect the circle of radius 2 in at most two places (unless $a = b$, which is ruled out by $a \nparallel b$), it follows that $\gamma = \pm 1$. The case $a = -c$ is similar. □

Proof of Proposition 5.1.5. By Remark 5.1.2, it suffices to find all maximal antipodal sets containing $[I]$ and $[U]$, where $U = F(\alpha)$ for some α of modulus one. If a frame $[V]$ is antipodal from $[I]$, Proposition 5.0.5 shows that V may be written as $V = \sigma h F(\beta)$ for some $\beta \in U_1$, diagonal unitary h, and permutation $\sigma \in S_4$. Furthermore, we may assume that σ fixes e_1. (This is because for any permutation $\tau \in S_4$, there exists a diagonal unitary g and a permutation $\rho \in S_4$ which fixes e_1 such that $\tau F(\beta) = \rho F(\gamma) g$, where $\gamma = \beta$ or $\bar{\beta}$).

If $[V]$ is also antipodal from $[U]$ then we must have $os(U^* V) = J_4$, so if $h = \mathrm{diag}(a, b, c, d)$, the matrix given by

$$\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & \bar{\alpha} & -\bar{\alpha} \\ 1 & -1 & -\bar{\alpha} & \bar{\alpha} \end{pmatrix} \sigma \begin{pmatrix} a & a & a & a \\ b & b & -b & -b \\ c & -c & c\beta & -c\beta \\ d & -d & -d\beta & d\beta \end{pmatrix}$$

has entries of modulus 2.

If the (j, k) entry of $\sigma h F(\beta)$ is denoted by a_{jk}, it follows that

$$\begin{aligned} |a_{1j} + a_{2j} + a_{3j} + a_{4j}| &= 2 \\ |a_{1j} + a_{2j} - a_{3j} - a_{4j}| &= 2 \\ |a_{1j} - a_{2j} + \bar{\alpha} a_{3j} - \bar{\alpha} a_{4j}| &= 2 \\ |a_{1j} - a_{2j} - \bar{\alpha} a_{3j} + \bar{\alpha} a_{4j}| &= 2 \end{aligned} \tag{5.7}$$

for all column indices $j = 1, \ldots, 4$.

The first equation with $j = 1, 2$ shows that a, b, c, d satisfy the hypotheses of Lemma 5.1.6, while setting $j = 3$ gives exactly the equation in Lemma 5.1.8 if we set $\gamma = \beta$. Thus either $a \parallel b$ or $\beta = \pm 1$.

There are now three cases to consider.

1. $\sigma(e_2) = e_2$

   The third and fourth equations in (5.7) with $j = 1$ show that $|a-b+\bar{\alpha}c-\bar{\alpha}d| = 2$. Applying Lemma 5.1.8 with $\gamma = \bar{\alpha}$ shows that $a \parallel b$ or $\alpha = \pm 1$.

2. $\sigma(e_3) = e_2$

   The third and fourth equations in (5.7) with $j = 1$ show that $|a-c+\bar{\alpha}b-\bar{\alpha}d| = 2$. Lemma 5.1.8 applies with $\gamma = \bar{\alpha}$ to show that $a \parallel c$ or $\alpha = \pm 1$.

3. $\sigma(e_4) = e_2$

   The third and fourth equations in (5.7) with $j = 1$ show that $|a-d+\bar{\alpha}b-\bar{\alpha}c| = 2$. Lemma 5.1.8 applies with $\gamma = \bar{\alpha}$ to show that $a \parallel d$ or $\alpha = \pm 1$.

If $\alpha \neq \pm 1$ then, after checking the various possible cases, $[V]$ can be represented by $\operatorname{diag}(a, a, c, -c)\ F(\beta)$ for some a, c, β of modulus one.

Otherwise, $\alpha = \pm 1$. In this case, $[V]$ may still be represented by $\operatorname{diag}(a, a, c, -c)$ $F(\beta)$ for some a, c, β of modulus one, but it could also be represented by $\operatorname{diag}(a, b, c, d)$ $F(1)$ where two of a, b, c, d are equal and the other two sum to zero.

One can readily verify that in both cases, the possibilities touted for $[V]$ are indeed antipodal from both $[I]$ and $[F(\alpha)]$. Can we extend $\{[I], [F(\alpha)], [V]\}$ to a larger collection of mutually antipodal frames?

First suppose $\alpha \neq \pm 1$, and suppose $[V]$ and $[W]$ are antipodal from $[I]$ and $[F(\alpha)]$; thus $[V]$ and $[W]$ can be represented by

$$V = \operatorname{diag}(a, a, c, -c)F(\beta), W = \operatorname{diag}(b, b, d, -d)F(\gamma),$$

respectively. If $[V]$ and $[W]$ are antipodal then $os(W^*V) = J_4$; this implies that the frames represented by $F(\gamma)$ and $\operatorname{diag}(\bar{b}a, \bar{b}a, \bar{d}c, \bar{d}c)F(\beta)$ are antipodal. Note the second frame is also antipodal from $[I]$. But we have just seen that for a frame to be antipodal from both $[I]$ and $F(\gamma)$, it must have the form $\operatorname{diag}(p, q, r, s)F(\delta)$ where two of p, q, r, s are equal and the other two sum to zero. Since $(\bar{b}a, \bar{b}a, \bar{d}c, \bar{d}c)$ does not satisfy this condition it follows that $[V]$ and $[W]$ cannot be antipodal, so $\{[I], [F(\alpha)], [\operatorname{diag}(a, a, c, -c)F(\beta)]\}$ is a maximal antipodal set. This proves the first assertion of the proposition.

For the second assertion, suppose $\alpha = \pm 1$ (since $[F(1)] = [F(-1)]$ we can assume $\alpha = 1$). Suppose $[V]$ and $[W]$ are antipodal from each other and from both $[I]$ and $[F(\alpha)] = [F(1)]$; thus $[V]$ and $[W]$ can be represented by

$$V = \operatorname{diag}(a, b, c, d)F(1), W = \operatorname{diag}(\bar{w}, \bar{x}, \bar{y}, \bar{z})F(1),$$

respectively, where two of a, b, c, d are equal and the other two sum to zero (and similarly for w, x, y, z). (The case of $[V]$ represented by $\text{diag}(a, a, c, -c)F(\beta)$ for some $\beta \neq \pm 1$ need not be considered, since that has already been covered by the first assertion of the proposition.)

That $[V]$ and $[W]$ are antipodal implies $os(W^*V) = J_4$, whence the frames represented by $F(1)$ and $\text{diag}(wa, xb, yc, zd)F(1)$ are antipodal. Thus two of wa, xb, yc, zd are equal and the other two sum to zero.

Consideration of all possible cases shows that $[V], [W]$ must be represented by one of $\text{diag}(1, 1, i, -i)F(1)$, $\text{diag}(1, i, -i, 1)F(1)$, or $\text{diag}(1, -i, 1, i)F(1)$. Since all three of these unitaries represent frames which are antipodal from both $[I]$,$[F(1)]$ and from each other, the second assertion of the proposition follows. □

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