Optimal Tight Frames and Quantum Measurement

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Abstract

Tight frames and rank-one quantum measurements are shown to be intimately related. In fact, the family of normalized tight frames for the space in which a quantum mechanical system lies is precisely the family of rank-one generalized quantum measurements (POVMs) on that space. Using this relationship, frame-theoretical analogues of various quantum-mechanical concepts and results are developed.

The analogue of a least-squares quantum measurement is a tight frame that is closest in a least-squares sense to a given set of vectors. The least-squares tight frame is found for both the case in which the scaling of the frame is specified (constrained least-squares frame (CLSF)) and the case in which the scaling is free (unconstrained least-squares frame (ULSF)). The well-known canonical frame is shown to be proportional to the ULSF and to coincide with the CLSF with a certain scaling.

Finally, the canonical frame vectors corresponding to a geometrically uniform vector set are shown to be geometrically uniform and to have the same symmetries as the original vector set.

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1 Introduction

Frames are generalizations of bases which lead to redundant signal expansions [1, 2]. A frame for a Hilbert space $\mathcal{U}$ is a set of not necessarily linearly independent vectors that spans $\mathcal{U}$ and has some additional properties. Frames were first introduced by Duffin and Schaeffer [1] in the context of nonharmonic Fourier series, and play an important role in the theory of nonuniform sampling [1, 2, 3]. Recent interest in frames has been motivated in part by their utility in analyzing wavelet expansions [4, 5].

Many efforts have been made to construct bases with specified properties. Since the conditions on bases are quite stringent, in many applications it is hard to find “good” bases. The conditions on frame vectors are usually not as stringent, allowing for increased flexibility in their design [4, 6]. For example, frame expansions admit signal representations that are localized in both time and frequency [3], as well as sparse representations [7].

Frame expansions have many other desirable properties. The coefficients may be computed with less precision than the coefficients in a basis expansion for a given desired reconstruction precision [5]; the effect of additive noise on the coefficients on the reconstructed signal is reduced in comparison with a basis expansion [3, 8, 9, 10]; and the coefficients are more robust to quantization degradations [11, 12]. Recently, frames have been applied to the development of modern uniform and nonuniform sampling techniques [13], to various detection problems [14, 15], and to the analysis and design of packet-based communication systems [16].

A tight frame is a special case of a frame for which the reconstruction formula is particularly simple. As we show in Section 4, a tight frame expansion of a signal is reminiscent of an orthogonal basis expansion, even though the frame vectors in the expansion are linearly dependent. Tight frames are particularly popular, and will be the focus of this paper.

Frame-like expansions have been developed and used in a wide range of disciplines. Many connections between frame theory and various signal processing techniques have been recently
discovered and developed. For example, the theory of frames has been used to analyze and design oversampled filter banks [17, 18] and error correction codes [19]. Wavelet families have been used in quantum mechanics and many other areas of theoretical physics, particularly in the study of semiclassical approximations to quantum mechanics [5].

In this paper we explore yet another connection between quantum mechanics and tight frames. Specifically, we show that the family of (normalized) tight frames for a subspace $U$ in which a quantum mechanical system is known to lie is precisely the family of possible generalized measurements (POVMs) on $U$. Exploiting this equivalence, we can apply ideas and results derived in the context of quantum measurement to the theory of frames and vice versa.

We begin in Section 3 by characterizing quantum measurements. With each rank-one quantum measurement we associate a measurement matrix. Using the measurement matrix representation, we give a simple and constructive proof of Neumark’s theorem [20], which relates general quantum measurements to orthogonal measurements. We then discuss the problem of constructing measurements optimized to distinguish between a set of non-orthogonal pure quantum states.

We then follow a similar path in Section 4 for tight frames. We associate a frame matrix with every tight frame, which as we show has essentially the same properties as a quantum measurement matrix. Next, we derive an analogue of Neumark’s theorem for tight frames, which expresses tight frame vectors as projections of a set of orthogonal vectors in a larger space. Finally, motivated by the construction of optimal quantum measurements, we consider the problem of constructing optimal tight frames for a subspace $U$ from a given set of vectors that span $U$.

The problem of frame design has received relatively little attention in the frame literature. Typically in applications the frame vectors are chosen, rather than optimized. Iterative algorithms for constructing frames that are optimal in some sense are given in [21]. Methods for generating frames starting from a given frame are described in [6].

A popular frame construction from a given set of vectors is the canonical frame [8–17, 22, 24],
first proposed in the context of wavelets in [24]. The canonical frame is relatively simple to construct, can be determined directly from the given vectors, and plays an important role in wavelet theory [25, 26, 27]. However, no general optimality properties are known for the canonical frame.

In Section 5 we systematically construct optimal frames from a given set of vectors. Motivated by the least-squares measurement [28] derived for quantum detection, we seek a tight frame consisting of frame vectors that minimize the sum of the squared norms of the error vectors, where the $i$th error vector is defined as the difference between the $i$th given vector and the $i$th frame vector. We consider both the case in which the scaling of the frame is specified, and the case in which the scaling is such that the error is minimized. When the scaling is specified the optimizing frame is referred to as the constrained least-squares frame (CLSF), and when the scaling is not specified the optimizing frame is referred to as the unconstrained least-squares frame (ULSF).

In Section 7 we show that the canonical frame vectors are proportional to the ULSF vectors, and that they coincide with the CLSF vectors with a specific choice of scaling.

An important issue is to what extent frames constructed from a given set of vectors inherit the properties of the original vector set [22]. For example, it has been shown that when constructing normalized Gabor frames from windows satisfying certain decay conditions using the canonical frame construction, the resulting tight frame has similar decay properties [22]. In Section 8 we consider the case in which the original vectors have a strong symmetry property called geometric uniformity [29]. Based on results derived in the context of quantum detection [28] we show that the CLSF vectors and the ULSF vectors have the same symmetries as the original vectors. This implies that the canonical frame vectors associated with a geometrically uniform vector set are themselves geometrically uniform.

Before proceeding to the detailed development, in Section 2 we first provide an overview of the notation and some mathematical preliminaries.
2 Preliminaries

In this section we briefly review elements of linear algebra that are common to both signal processing and quantum mechanics. Our main goal is to characterize “transjectors” (partial isometries) using the singular value decomposition (SVD).

2.1 Hilbert spaces and operators

In both signal processing and quantum mechanics, the setting we consider is a finite-dimensional subspace $\mathcal{U}$ of a complex Hilbert space $\mathcal{H}$. The elements of $\mathcal{H}$ are called vectors. We will often assume for notational convenience that $\mathcal{H}$ is finite-dimensional, with $\dim \mathcal{H} = k$; then by appropriate choice of coordinates we can identify $\mathcal{H}$ with $\mathbb{C}^k$.

In signal processing, the elements of $\mathcal{H}$ are regarded as column vectors and denoted, e.g., by $x \in \mathcal{H}$. Then $x^*$ denotes the row vector which is the conjugate transpose of $x$. The inner product of two vectors is a complex number, denoted, e.g., by $\langle x, y \rangle = x^*y$. An outer product of two vectors such as $xy^*$ is a rank-one matrix, which as an operator takes $z \in \mathcal{H}$ to $xy^*z = \langle y, z \rangle x \in \mathcal{H}$.

The Dirac bra-ket notation of quantum mechanics expresses such concepts very nicely. We believe that the signal processing community would do well to master it; however, recognizing that it is unfamiliar, we do not rely on it in this paper. Nonetheless, to assist the reader unfamiliar with this notation in reading the quantum literature, we will give the bra-ket equivalents for various expressions in this section.

In the bra-ket notation, the elements of $\mathcal{H}$ are “ket” vectors, denoted, e.g., by $|x\rangle \in \mathcal{H}$. The corresponding “bra” vector $\langle x|$ is an element of the dual space $\mathcal{H}^*$ and may be regarded as the conjugate transpose of $|x\rangle$. The inner product of two vectors is a complex number denoted by $\langle x|y \rangle$. An outer product of two vectors such as $|x\rangle\langle y|$ is a rank-one matrix, which as an operator takes $|z\rangle \in \mathcal{H}$ to $|x\rangle\langle y||z\rangle = \langle y|z\rangle |x\rangle \in \mathcal{H}$.

An operator on $\mathcal{H}$ is a linear transformation $A : \mathcal{H} \to \mathcal{H}$. The adjoint of an operator $A$ is the
unique operator $A^*$ such that $\langle x, Ay \rangle = \langle A^*x, y \rangle$ for all $x, y \in \mathcal{H}$. If the elements of $\mathcal{H}$ are column vectors, then an operator $A$ is represented by a square matrix, and its adjoint is represented by the conjugate transpose $A^*$, since $\langle x, Ay \rangle = x^*Ay = (A^*x)^*y = \langle A^*x, y \rangle$.

An operator $A$ is called Hermitian if it is self-adjoint; i.e., if $A^* = A$.

An orthogonal projector $P$ is a Hermitian operator on $\mathcal{H}$ such that $P^2 = P$. Consequently, the eigenvalues of $P$ all equal 0 or 1. If $\{u_i\}$ is a set of eigenvectors corresponding to the nonzero eigenvalues of $P$, then the subspace $\mathcal{U} \subseteq \mathcal{H}$ spanned by the set $\{u_i\}$ is the range of $P$, and we write the projector as $P_\mathcal{U}$. A one-dimensional projector has a single eigenvector $u$ and may be written as the outer product $P u = uu^*$ (or $P u = |u\rangle\langle u|$ in bra-ket notation); then $P u$ projects any $x \in \mathcal{H}$ into the projection $P u x = \langle u, x \rangle u$ (or $|u\rangle\langle u| x \rangle$). An $r$-dimensional projector $P_\mathcal{U}$ may be written as the sum of $r$ one-dimensional projectors, $P_\mathcal{U} = \sum_i P_{u_i}$, where $\{u_i\}$ is any basis for $\mathcal{U}$.

2.2 Transjectors (partial isometries)

Let $F$ be a rank-$r$ matrix whose columns are a set of $n$ vectors $\varphi_i \in \mathcal{H}$. Then $F^*x$ is a vector in $\mathbb{C}^n$ whose components are the inner products $\langle \varphi_i, x \rangle$. In other words, $F^*$ may be regarded as a linear transformation $F^* : \mathcal{H} \to \mathbb{C}^n$. Similarly, $F$ may be regarded as a linear transformation $F : \mathbb{C}^n \to \mathcal{H}$.

It is well known in signal processing (but not as well known in quantum mechanics) that any such matrix $F$ has an SVD $F = U \Sigma V^*$, where $U$ is a unitary matrix whose columns $\{u_i \in \mathcal{H}\}$ are the eigenvectors of the Hermitian operator $T = FF^*$, $V$ is a unitary matrix whose columns $\{v_i \in \mathbb{C}^n\}$ are the eigenvectors of the Hermitian matrix $S = F^*F$ (the Gram matrix of inner products), and $\Sigma$ is a positive real diagonal matrix whose $r$ nonzero values $\sigma_i$, called the singular values of $F$, are the positive square roots of the nonzero eigenvalues of either $S$ or $T$. Thus we may write $F = \sum_i \sigma_i u_i v_i^*$ (or $F = \sum_i \sigma_i |u_i\rangle\langle v_i|$), a sum of $r$ rank-1 outer products.

An outer product such as $u_i v_i^*$ (or $|u_i\rangle\langle v_i|$) is called a one-dimensional transjector. The trans-
jector $u_i v_i^*$ takes a basis vector $v_i \in \mathbb{C}^n$ to the corresponding basis vector $u_i \in \mathcal{H}$. By linear superposition, it therefore takes a general element $x = \sum_j \langle v_j, x \rangle v_j \in \mathbb{C}^n$ to $u_i v_i^* x = \langle v_i, x \rangle u_i \in \mathcal{H}$. Similarly, the adjoint transjector $v_i u_i^*$ takes $y = \sum_j \langle u_j, y \rangle u_j \in \mathcal{H}$ to $v_i u_i^* y = \langle u_i, y \rangle v_i \in \mathbb{C}^n$.

The subspace spanned by the $r$ eigenvectors $u_i \in \mathcal{H}$ corresponding to the $r$ nonzero eigenvalues of $S = F^* F$ will be denoted as $U \subseteq \mathcal{H}$, and the subspace spanned by the $r$ eigenvectors $v_i \in \mathbb{C}^n$ corresponding to the $r$ nonzero eigenvalues of $T = F F^*$ will be denoted as $V \subseteq \mathbb{C}^n$. The image of $F$ is $U$, and the image of $F^*$ is $V$; the kernel of $F$ is the orthogonal complement $V^\perp$ of $V$, and the kernel of $F^*$ is $U^\perp$. $F$ operates by first performing an orthonormal expansion of $\mathbb{C}^n$ using the basis $\{v_i\}$, scaling each component by $\sigma_i$, and then “transjecting” to $U \subseteq \mathcal{H}$ by replacing each $v_i$ by the corresponding $u_i$. $F^*$ similarly “transjects” from $\mathcal{H}$ to $V \subseteq \mathbb{C}^n$.

A rank-$r$ matrix $F$ is called an $r$-dimensional transjector if its $r$ nonzero singular values are all equal to 1. In other words, $F = UZ_r V^*$, where $U$ and $V$ are unitary and

$$Z_r = \begin{bmatrix} I_r & 0 \\ 0 & 0 \end{bmatrix}. \quad (1)$$

Equivalently, $F F^* = U(Z_r Z_r^*) U^* = P_U$ is an $r$-dimensional orthogonal projector onto an $r$-dimensional subspace $U \subseteq \mathcal{H}$ with an orthonormal basis $\{u_i \in \mathcal{H}, 1 \leq i \leq r\}$ (the $U$-basis) consisting of the first $r$ columns of $U$, and $F^* F = V(Z_r^* Z_r) V^* = P_V$ is an $r$-dimensional orthogonal projector onto an $r$-dimensional subspace $V \subseteq \mathbb{C}^n$ with an orthonormal basis $\{v_i \in \mathbb{C}^n, 1 \leq i \leq r\}$ (the $V$-basis) consisting of the first $r$ columns of $V$.

The SVD $F = UZ_r V^*$ thus reduces to a sum of $r$ one-dimensional transjectors (outer products):

$$F = \sum_{i=1}^r u_i v_i^*. \quad (2)$$
If $u \in \mathcal{U}$, then $u = \sum_{i=1}^{r} (u, u) u_i$, and

$$F^* u = \sum_{i=1}^{r} (u, u) v_i;$$

(3)

i.e., $F^*$ “transjects” $u$ to a corresponding vector $v \in \mathcal{V}$. Similarly, if $v \in \mathcal{V}$, then

$$Fv = \sum_{i=1}^{r} (v, v) u_i;$$

(4)

i.e., $F$ performs the inverse map from $\mathcal{V}$ to $\mathcal{U}$. If $u \in \mathcal{H}$, then $F^*$ first projects $u$ onto $\mathcal{U}$ and then “transjects” to $\mathcal{V}$ as above; similarly, for a general $v \in \mathbb{C}^n$, $F$ first projects $v$ onto $\mathcal{V}$ and then “transjects” to $\mathcal{U}$ as above.

An $r$-dimensional transjector $F$ is also called a partial isometry, because it is an isometry (distance-preserving transformation) between the subspaces $\mathcal{U} \subseteq \mathcal{H}$ and $\mathcal{V} \subseteq \mathbb{C}^n$. Indeed, if $v, v' \in \mathcal{V}$ and $u = Fv, u' = Fv'$, then

$$\langle u, u' \rangle = u^* u' = v^* F^* F v' = v^* P_{\mathcal{V}} v' = v^* v' = \langle v, v' \rangle,$$

(5)

so inner products and a fortiori squared norms and distances are preserved. Similarly, if $u, u' \in \mathcal{U}$, then $\langle F^* u, F^* u' \rangle = \langle u, u' \rangle$. However, inner products are not preserved if $u, u' \in \mathcal{U}$ or $v, v' \in \mathcal{V}$.

This discussion is summarized in the following theorem:

**Theorem 1 (Transjectors (partial isometries)).** The following statements are equivalent for a matrix $F$ whose columns are $n$ vectors in a complex Hilbert space $\mathcal{H}$:

1. $F$ is a transjector (partial isometry) between $r$-dimensional subspaces $\mathcal{U} \subseteq \mathcal{H}$ and $\mathcal{V} \subseteq \mathbb{C}^n$;

2. $FF^* = P_{\mathcal{U}}$ for an $r$-dimensional subspace $\mathcal{U} \subseteq \mathcal{H}$;

3. $F^* F = P_{\mathcal{V}}$ for an $r$-dimensional subspace $\mathcal{V} \subseteq \mathbb{C}^n$. 

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A transjector $F$ between $r$-dimensional subspaces $U \subseteq \mathcal{H}$ and $V \subseteq \mathbb{C}^n$ may be expressed as $F = UZ_rV^*$, where $U$ is a unitary matrix whose first $r$ columns $\{u_i, 1 \leq i \leq r\}$ are an orthonormal basis for $U$, $V$ is an $n \times n$ unitary matrix whose first $r$ columns $\{v_i, 1 \leq i \leq r\}$ are an orthonormal basis for $V$, and $Z_r$ is given by (1). Equivalently, $F = \sum_{i=1}^{r} u_i v_i^*$.

A transjector $F : \mathbb{C}^n \to U$ (resp. $F^* : \mathcal{H} \to V$) is an isometry if restricted to $V$ (resp. $U$).

3 Quantum Measurement

In this section we present some elements of the theory of quantum measurement, following [28] and unpublished work in [30]. In the remainder of the paper we will develop analogous results for tight frames.

A quantum system in a pure state is characterized by a normalized vector $\phi$ in a Hilbert space $\mathcal{H}$. Information about a quantum system is extracted by subjecting the system to a measurement. In quantum theory, the outcome of a measurement is inherently probabilistic, with the probabilities of the outcomes of any conceivable measurement determined by the state vector $\phi \in \mathcal{H}$.

A quantum measurement is described by a collection of Hermitian operators $\{Q_i\}$ on $\mathcal{H}$, where the index $i$ corresponds to a possible measurement outcome. The laws of quantum mechanics impose certain mathematical constraints on the measurement operators.

In the simplest case, the measurement operators are rank-one operators and have the outer-product form $Q_i = \mu_i \mu_i^*$ for some nonzero vectors $\mu_i \in \mathcal{H}$. Such measurements will be called rank-one measurements, and the vectors $\mu_i$ will be called the measurement vectors.

If the state vector is $\phi$, then the probability of observing the $i$th outcome is

$$p(i) = \langle \phi, Q_i \phi \rangle = |\langle \mu_i, \phi \rangle|^2.$$  (6)
To ensure that the probabilities $p(i)$ sum to 1 for any normalized $\phi \in \mathcal{H}$, we impose the constraint
\[
\sum_i Q_i = I_{\mathcal{H}},
\]
where $I_{\mathcal{H}}$ is the identity operator on $\mathcal{H}$; then
\[
\sum_i p(i) = \langle \phi, \sum_i Q_i \phi \rangle = \langle \phi, \phi \rangle = 1.
\]

We distinguish between standard (von Neumann) measurements and generalized measurements, or positive operator-valued measures (POVMs). In a standard measurement, the measurement operators $\{Q_i\}$ form a complete set of orthogonal projectors. Thus
\[
Q_i Q_i = Q_i; \quad (9)
\]
\[
Q_i Q_j = 0, \quad \text{if } i \neq j; \quad (10)
\]
\[
\sum_i Q_i = I_{\mathcal{H}}. \quad (11)
\]
If the measurement is rank-one, so that $Q_i = \mu_i \mu_i^*$, then (9) and (10) imply that $\langle \mu_i, \mu_j \rangle = \delta_{ij}$, while (11) implies that
\[
x = I_{\mathcal{H}} x = \sum_i \langle \mu_i, x \rangle \mu_i, \quad \forall x \in \mathcal{H},
\]
so the measurement vectors $\{\mu_i\}$ form an orthonormal basis for $\mathcal{H}$.

Sometimes a generalized measurement is a more efficient way of obtaining information about the state of a quantum system than a standard measurement [20]. A generalized measurement consists of a set $\{Q_i\}$ of nonnegative Hermitian operators, not necessarily projectors, that satisfy $\sum_i Q_i = I_{\mathcal{H}}$. Such a set of operators is termed a POVM. If the measurement is rank-one so that
\[ Q_i = \mu_i \mu_i^*, \text{ then the measurement vectors } \mu_i \text{ must satisfy} \]
\[ \sum_i \mu_i \mu_i^* = I_{\mathcal{H}}. \]  
(13)

A POVM is more general than a standard measurement in that the measurement vectors \( \mu_i \) are not required to be either normalized or orthogonal.

It can be shown that a generalized measurement on a quantum system can be implemented by introducing an auxiliary system and performing standard measurements on the combined system. We will discuss this property in Section 3.2 in the context of Neumark’s theorem; in Section 4.2 we show that this property has an analogue for tight frames.

### 3.1 Measurement Matrices

A rank-one POVM acting on an \( r \)-dimensional subspace \( \mathcal{U} \subseteq \mathcal{H} \) in which the system to be measured is known \textit{a priori} to lie is defined by a set of \( n \) measurement vectors \( \{\mu_i, 1 \leq i \leq n\} \) that satisfy

\[ \sum_{i=1}^{n} \mu_i \mu_i^* = P_{\mathcal{U}}, \]  
(14)

\textit{i.e.,} the \( n \) operators \( Q_i = \mu_i \mu_i^* \) must be a resolution of the identity on \( \mathcal{U} \).

The \textit{measurement matrix} \( M \) corresponding to a set of measurement vectors \( \mu_i \in \mathcal{U} \) is defined as the matrix of columns \( \mu_i \). We have immediately from (14) that

\[ MM^* = P_{\mathcal{U}}. \]  
(15)

Thus a matrix \( M \) with \( n \) columns in \( \mathcal{H} \) is a measurement matrix for states in the subspace \( \mathcal{U} \subseteq \mathcal{H} \) if and only if \( M \) satisfies (15).

\[ ^1\text{Often these operators are supplemented by a projection } Q_0 = P_{\mathcal{U}^\perp} = I_{\mathcal{H}} - P_{\mathcal{U}} \text{ onto the orthogonal subspace } \mathcal{U}^\perp \subseteq \mathcal{H}, \text{ so that } \sum_{i=0}^{n} Q_i = I_{\mathcal{H}} \text{ i.e., the augmented POVM is a resolution of the identity on } \mathcal{H}. \]
It follows immediately from Theorem 1 that a measurement matrix $M$ with $n$ columns in $\mathcal{H}$ corresponds to a rank-one POVM acting on an $r$-dimensional subspace $\mathcal{U} \subseteq \mathcal{H}$ if and only if $M$ is a transjector (partial isometry) between $\mathcal{U}$ and an $r$-dimensional subspace $\mathcal{V} \subseteq \mathbb{C}^n$. Thus $M$ has all the properties enumerated in Theorem 1.

A measurement matrix $M$ represents a standard measurement if and only if its $n$ columns are orthonormal; i.e., if and only if its Gram matrix satisfies $M^*M = I_n$. Then $M$ has rank $n$, $\mathcal{U}$ has dimension $n$, $\mathcal{V} = \mathbb{C}^n$, and $M = UZ_nV^*$ for unitary $U$ and $V$, where $Z_n$ is given by

$$Z_n = \begin{bmatrix} I_n \\ 0 \end{bmatrix}.$$  \hspace{1cm} (16)

We summarize the properties of measurement matrices in the following theorem.

**Theorem 2 (Measurement matrices).** The following statements are equivalent for a matrix $M$ whose columns are $n$ vectors in a complex Hilbert space $\mathcal{H}$:

1. $M$ is a measurement matrix corresponding to a rank-one POVM acting on an $r$-dimensional subspace $\mathcal{U} \subseteq \mathcal{H}$;

2. $M$ is a transjector (partial isometry) between $r$-dimensional subspaces $\mathcal{U} \subseteq \mathcal{H}$ and $\mathcal{V} \subseteq \mathbb{C}^n$;

3. $MM^* = P_{\mathcal{U}}$ for an $r$-dimensional subspace $\mathcal{U} \subseteq \mathcal{H}$;

4. $M^*M = P_{\mathcal{V}}$ for an $r$-dimensional subspace $\mathcal{V} \subseteq \mathbb{C}^n$.

A measurement matrix $M$ corresponding to a rank-one POVM acting on an $r$-dimensional subspace $\mathcal{U} \subseteq \mathcal{H}$ may be expressed as $M = UZ_rV^*$, where $U$ is a unitary matrix whose first $r$ columns $\{u_i, 1 \leq i \leq r\}$ are an orthonormal basis for $\mathcal{U}$, $V$ is an $n \times n$ unitary matrix whose first $r$ columns $\{v_i, 1 \leq i \leq r\}$ are an orthonormal basis for $\mathcal{V}$, and $Z_r$ is given by (16). Equivalently, $M = \sum_{i=1}^r u_i v_i^*$. 

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A measurement matrix \( M \) is an isometry if restricted to \( V \).

A measurement matrix \( M \) whose columns are \( n \) vectors in \( \mathcal{H} \) represents a standard measurement if and only if its rank is \( n \). Then \( M = UZ_nV^* \), where \( Z_n \) is given by (14), and \( M^*M = I_n \).

### 3.2 Neumark’s Theorem

Neumark’s theorem \[20\] guarantees that any POVM with measurement vectors \( \mu_i \in \mathcal{U} \) can be realized by a set of orthonormal vectors \( \tilde{\mu}_i \) in an extended space \( \tilde{\mathcal{U}} \) such that \( U \subseteq \tilde{\mathcal{U}} \), so that \( \mu_i = P_U\tilde{\mu}_i \).

Using the measurement matrix characterization of a POVM and the SVD, we now obtain a simple statement and proof of Neumark’s theorem. Moreover, our proof is constructive; we explicitly construct a set of orthogonal measurement vectors such that their projections onto \( U \) are the original measurement vectors. In Section 4.2 we use this construction to extend a tight frame into an orthogonal basis for a larger space.

**Theorem 3 (Neumark’s theorem).** Let \( M \) be a rank-\( r \) measurement matrix of an arbitrary POVM, with \( n \) columns in a complex Hilbert space \( \mathcal{H} \). In other words, \( M \) is a transjector between an \( r \)-dimensional subspace \( U \subseteq \mathcal{H} \) and an \( r \)-dimensional subspace \( V \subseteq \mathbb{C}^n \). Then there exists a standard (von Neumann) measurement with measurement matrix \( \tilde{M} \) which is a transjector between an expanded \( n \)-dimensional subspace \( \tilde{U} \supseteq U \) in a possibly expanded complex Hilbert space \( \tilde{\mathcal{H}} \supseteq \mathcal{H} \) and \( \mathbb{C}^n \), and whose projection onto \( U \) is \( M = P_U\tilde{M} \).

**Proof.** Using Theorem \[2\] we may express \( M \) as \( M = UZ_rV^* \). Let \( u_i \) and \( v_i \) denote the columns of \( U \) and \( V \) respectively. Assume that \( \mathcal{H} \) is finite-dimensional, and let \( k = \dim \mathcal{H} \).

We distinguish between the case \( k \geq n \) (i.e., \( M \) has at least as many rows as columns), and the case \( k < n \) (i.e., \( M \) has more columns than rows).

In the case \( k \geq n \), define \( \tilde{M} = \sum_{i=1}^{n} u_iv_i^* \); then \( \tilde{U} \subseteq \mathcal{H} \) is the \( n \)-dimensional subspace spanned
by \( \{ u_i, 1 \leq i \leq n \} \). The projection of \( \widetilde{M} \) onto \( \mathcal{U} \) is

\[
P_{\mathcal{U}} \widetilde{M} = \sum_{j=1}^{m} u_j u_j^* \sum_{i=1}^{n} u_i v_i^* = \sum_{i=1}^{m} u_i v_i^* = M. \tag{17}
\]

Moreover, the columns of \( \widetilde{M} \) are orthonormal, since its Gram matrix is

\[
\widetilde{M}^* \widetilde{M} = \sum_{j=1}^{n} v_j v_j^* \sum_{i=1}^{n} u_i v_i^* = \sum_{i=1}^{n} v_i v_i^* = I_n. \tag{18}
\]

In the case \( k < n \), first embed \( \mathcal{U} \) in an \( n \)-dimensional space \( \tilde{\mathcal{U}} \) in an expanded complex Hilbert space \( \tilde{\mathcal{H}} \supseteq \mathcal{H} \), and let \( \{ \tilde{u}_i, 1 \leq i \leq n \} \) be an orthonormal basis for \( \tilde{\mathcal{U}} \) of which the first \( m \) vectors are the \( \mathcal{U} \)-basis. Then proceed as before, using \( \tilde{u}_i \) in place of \( u_i \).

It is instructive to consider the matrix representation of \( \widetilde{M} \) in both cases. Recall that \( M = UZ_rV^* \), where \( Z_r \) is given by (1).

In the case \( k \geq n \), we construct \( \widetilde{M} \) simply by extending the identity matrix along the diagonal; thus \( \widetilde{M} = UZ_nV^* \) where \( Z_n \) is given by (10). Thus, when \( k \geq n \), the left and right unitary matrices in the SVD of \( M \) and \( \widetilde{M} \) are the same, and are equal to \( U \) and \( V \), respectively.

If \( k = n \), then \( Z_n = I_n \) and \( \widetilde{M} = UV^* \).

In the case \( k < n \), we first replace the left unitary matrix \( U \) by \( \tilde{U} \), and thus replace \( k \) by \( \tilde{k} = n \); then \( \tilde{U} \) is an \( n \times n \) unitary matrix whose first \( r \) columns are the \( \mathcal{U} \)-basis (where we append \( n - k \) zeros to each basis vector \( u_i \)). We then define \( \widetilde{M} = \tilde{U}V^* \).

Examples of the construction of the orthogonal measurement vectors associated with a given POVM along the lines of this proof will be given in Section 4.2, in the context of frames.
3.3 Optimal Quantum Measurements

We now recapitulate some results on optimal quantum measurements according to various criteria, which will be relevant to the construction of optimal tight frames.

Let \( \{\phi_i, 1 \leq i \leq n\} \) be a collection of \( n \leq k \) normalized vectors \( \phi_i \) in a \( k \)-dimensional complex Hilbert space \( \mathcal{H} \), representing different preparations of a quantum system. In general these vectors are non-orthogonal and span an \( r \)-dimensional subspace \( \mathcal{U} \subseteq \mathcal{H} \). The vectors are linearly independent if \( r = n \).

To distinguish between the different preparations, we subject the system to a measurement. For our measurement, we restrict our attention to POVMs consisting of \( n \) rank-one operators of the form \( Q_i = \mu_i \mu_i^* \) with measurement vectors \( \mu_i \in \mathcal{U} \). We do not require the vectors \( \mu_i \) to be orthogonal or normalized. However, to constitute a POVM on \( \mathcal{U} \) the measurement vectors must satisfy (14).

If the states are prepared with equal prior probabilities, then the probability of detection error using the measurement vectors \( \mu_i \) is given from (6) by

\[
P_e = 1 - \frac{1}{n} \sum_{i=1}^{n} |\langle \mu_i, \phi_i \rangle|^2.
\]  

(19)

If the vectors \( \mu_i \) are orthonormal, then choosing \( \mu_i = \phi_i \) results in \( P_e = 0 \). However, if the given vectors are not orthonormal, then no measurement can distinguish perfectly between them. Therefore, a fundamental problem in quantum mechanics is to construct measurements optimized to distinguish between a set of non-orthogonal pure quantum states.

This problem may be formulated as a quantum detection problem, so that the measurement vectors are chosen to minimize the probability of detection error, or more generally, minimize the Bayes cost. Necessary and sufficient conditions for an optimum measurement minimizing the Bayes cost have been derived [31, 32, 33]. However, except in some particular cases [33, 34, 35], obtaining
a closed-form analytical expression for the optimal measurement directly from these conditions is a difficult and unsolved problem.

An alternative approach proposed in [28] is to choose a different optimality criterion, namely a squared-error criterion, and to seek measurement vectors that minimize this criterion. Specifically, the measurement vectors are chosen to minimize the sum of the squared norms of the error vectors, where the $i$th error vector is defined as the difference between the $i$th state vector and the $i$th measurement vector. The optimizing measurement is referred to as the least-squares measurement (LSM).

It turns out that the LSM problem has a simple closed-form solution which has many desirable properties. Its construction is relatively simple; it can be determined directly from the given collection of states; it minimizes the probability of detection error when the states exhibit certain symmetries [28]; it is “pretty good” when the states to be distinguished are equally likely and almost orthogonal [36]; and it is asymptotically optimal [37].

In the next section we will develop a relationship between POVMs and tight frames. We then apply ideas and results derived in the context of quantum detection to the construction and characterization of tight frames. In particular, we will apply the squared-error criterion developed in [28] to the construction of optimal tight frames.
4 Tight Frames

Frames, which are generalizations of bases, were introduced in the context of nonharmonic Fourier series by Duffin and Schaeffer [1] (see also [2]). Recently, the theory of frames has been expanded [3, 4, 5, 8, 6], in part due to the utility of frames in analyzing wavelet decompositions. Here we will focus on tight frames, which have particularly nice properties.

Let \( \{\varphi_i, 1 \leq i \leq n\} \) denote a set of \( n \) vectors in an \( r \)-dimensional subspace \( \mathcal{U} \) of a Hilbert space \( \mathcal{H} \). The vectors \( \varphi_i \) form a tight frame for \( \mathcal{U} \) if there exists a constant \( \beta > 0 \) such that

\[
\sum_{i=1}^{n} |\langle x, \varphi_i \rangle|^2 = \beta^2 \|x\|^2,
\]

(20)

for all \( x \in \mathcal{U} \). If \( \beta = 1 \), the tight frame is said to be normalized; otherwise it is said to be \( \beta \)-scaled.

Of course any orthonormal basis for \( \mathcal{U} \) is a normalized tight frame for \( \mathcal{U} \). However, there also exist tight frames for \( \mathcal{U} \) with \( n > r \), which are necessarily linearly dependent. The redundancy of the tight frame is defined as \( \rho = n/r \).

Since

\[
\sum_{i=1}^{n} |\langle x, \varphi_i \rangle|^2 = \sum_{i=1}^{n} x^* \varphi_i \varphi_i^* x = \langle x, \left( \sum_{i=1}^{n} \varphi_i \varphi_i^* \right) x \rangle,
\]

(21)

More generally, the vectors \( \varphi_i \) form a frame for \( \mathcal{U} \) if there exist constants \( \alpha > 0 \) and \( \beta < \infty \) such that

\[
\alpha^2 \|x\|^2 \leq \sum_{i=1}^{n} |\langle x, \varphi_i \rangle|^2 \leq \beta^2 \|x\|^2,
\]

for all \( x \in \mathcal{U} \). The lower bound ensures that the vectors \( \varphi_i \) span \( \mathcal{U} \); thus we must have \( n \geq r \). If \( n < \infty \), then the right hand inequality is always satisfied with \( \beta^2 = \sum_{i=1}^{n} \langle \varphi_i, \varphi_i \rangle \). Thus, any finite set of vectors that spans \( \mathcal{U} \) is a frame for \( \mathcal{U} \). In particular, any basis for \( \mathcal{U} \) is a frame for \( \mathcal{U} \). However, in contrast to basis vectors, which are linearly independent, frame vectors with \( n > r \) are linearly dependent. A tight frame is a special case of a frame for which \( \alpha = \beta \).
the fact that (20) holds for all $x \in \mathcal{U}$ implies that

$$\sum_{i=1}^{n} \varphi_i \varphi_i^* = \beta^2 P_{\mathcal{U}}.$$  \hfill (22)

Conversely, if the vectors $\varphi_i \in \mathcal{U}$ satisfy (22), then (21) implies that (20) is satisfied for all $x \in \mathcal{U}$. We conclude that a set of $n$ vectors $\varphi_i \in \mathcal{U}$ forms a tight frame for $\mathcal{U}$ if and only if the vectors satisfy (22) for some $\beta > 0$.

Comparing (22) with (14), we conclude that:

**Theorem 4 (Tight frames).** A set of vectors $\varphi_i \in \mathcal{U}$ forms a $\beta$-scaled tight frame for $\mathcal{U}$ if and only if the scaled vectors $\beta^{-1} \varphi_i$ are the measurement vectors of a rank-one POVM on $\mathcal{U}$. In particular, the vectors $\varphi_i$ form a normalized tight frame for $\mathcal{U}$ if and only if they are the measurement vectors of a rank-one POVM on $\mathcal{U}$.

This fundamental relationship between rank-one quantum measurements and tight frames will be the basis for the developments in subsequent sections. In the next section, we define frame matrices in analogy to the measurement matrices of quantum mechanics. We then use Neumark’s theorem to extend tight frames to orthogonal bases. Motivated by the least-squares measurement of quantum mechanics, in Section 5 we address the problem of constructing optimal tight frames.
4.1 Frame Matrices

In analogy to the measurement matrix, we define the frame matrix $F$ as the matrix of columns $\varphi_i$, where the vectors $\varphi_i$ form a tight frame for $\mathcal{U}$. From (22) it then follows that

$$FF^* = \beta^2 P_{\mathcal{U}}. \quad (23)$$

The properties of a frame matrix $F$ follow immediately from Theorem 4 and Theorem 2:

**Theorem 5 (Frame matrices).** For a matrix $F$ whose columns are $n$ vectors in a complex Hilbert space $\mathcal{H}$ and for a constant $\beta > 0$, the following statements are equivalent:

1. $F$ is the frame matrix of a $\beta$-scaled tight frame for an $r$-dimensional subspace $\mathcal{U} \subseteq \mathcal{H}$;
2. $\beta^{-1} F$ is a transjector (partial isometry) between $r$-dimensional subspaces $\mathcal{U} \subseteq \mathcal{H}$ and $\mathcal{V} \subseteq \mathbb{C}^n$;
3. $FF^* = \beta^2 P_{\mathcal{U}}$ for an $r$-dimensional subspace $\mathcal{U} \subseteq \mathcal{H}$;
4. $F^*F = \beta^2 P_{\mathcal{V}}$ for an $r$-dimensional subspace $\mathcal{V} \subseteq \mathbb{C}^n$.

A frame matrix $F$ of a $\beta$-scaled tight frame for an $r$-dimensional subspace $\mathcal{U} \subseteq \mathcal{H}$ may be expressed as $F = \beta U Z_r V^*$, where $U$ is a unitary matrix whose first $r$ columns $\{u_i, 1 \leq i \leq r\}$ are an orthonormal basis for $\mathcal{U}$, $V$ is an $n \times n$ unitary matrix whose first $r$ columns $\{v_i, 1 \leq i \leq r\}$ are an orthonormal basis for $\mathcal{V}$, and $Z_r$ is given by (1). Equivalently, $F = \beta \sum_{i=1}^r u_i v_i^*$.

A frame matrix $F$ of a $\beta$-scaled tight frame is an isometry if restricted to $\mathcal{V}$ and scaled by $\beta^{-1}$.

A frame matrix $F$ of a $\beta$-scaled tight frame whose columns are $n$ vectors in $\mathcal{H}$ represents an orthogonal basis for $\mathcal{U}$ (i.e., is an orthogonal frame matrix) if and only if its rank is $n$. Then $F = \beta U Z_n V^*$, where $Z_n$ is given by (16), and $F^*F = \beta^2 I_n$; i.e., all frame vectors have squared norm $\beta^2$.

If the vectors $\{\varphi_i, 1 \leq i \leq n\}$ form a tight frame for $\mathcal{U}$, then any $x \in \mathcal{U}$ may be expressed as a linear combination of these vectors: $x = \sum_i a_i \varphi_i$. When $n > r$, the coefficients in this expansion
are not unique. A possible choice is \( a_i = \beta^{-2} \langle \varphi_i, x \rangle \), because

\[
\beta^{-2} \sum_{i=1}^{n} \langle \varphi_i, x \rangle \varphi_i = \beta^{-2} F F^* x = P_U x = x. \tag{24}
\]

This choice of coefficients has the property that among all possible coefficients it has the minimal norm \([8, 38]\).

The expansion of (24) is reminiscent of an expansion of \( x \) in terms of an orthonormal basis for \( U \). However, whereas the vectors in an orthonormal expansion are linearly independent, the vectors \( \varphi_i \) in (24) are linearly dependent when \( n > r \).

4.2 Neumark’s Theorem and Construction of Tight Frames

Neumark’s theorem (Theorem 3) was derived based on the properties of measurement matrices. Since by Theorem 4 frame matrices of tight frames have essentially the same properties as measurement matrices of rank-one POVMs, we can now obtain an equivalent of Neumark’s theorem for tight frames. The proof is essentially the same as the proof of Theorem 3, so we omit it.

**Theorem 6 (Neumark’s theorem for tight frames).** Let \( F \) be a rank-\( r \) frame matrix, with \( n \) columns in a complex Hilbert space \( \mathcal{H} \) that span an \( r \)-dimensional subspace \( \mathcal{U} \subseteq \mathcal{H} \). Then there exists an orthogonal frame matrix \( \tilde{F} \) with equal-norm orthogonal columns that span an expanded \( n \)-dimensional subspace \( \tilde{\mathcal{U}} \supseteq \mathcal{U} \) in a possibly expanded complex Hilbert space \( \tilde{\mathcal{H}} \supseteq \mathcal{H} \) such that the projection \( P_U \tilde{F} \) of \( \tilde{F} \) onto \( \mathcal{U} \) is \( F \).

We remark that given a set of equal-norm orthogonal vectors in \( \tilde{\mathcal{U}} \supseteq \mathcal{U} \), their projections onto \( \mathcal{U} \) will always form a tight frame for \( \mathcal{U} \) \([3]\). Combining this result with Theorem 3, we can conclude that a set of vectors forms a tight frame for \( \mathcal{U} \) if and only if the vectors can be expressed as a projection onto \( \mathcal{U} \) of a set of orthogonal vectors with equal norm in a larger space \( \tilde{\mathcal{U}} \) containing \( \mathcal{U} \).

Starting with a given frame matrix \( F \) in \( \mathcal{U} \), the proof of Theorem 3 gives a concrete construction
of an orthogonal frame matrix \( \tilde{F} \) in \( \tilde{U} \supseteq U \) such that \( P_\tilde{U} \tilde{F} = F \). We now give two examples of this construction. We consider first an example in which \( \dim \mathcal{H} < n \), and then one in which \( \dim \mathcal{H} > n \).

**Example 1.** Consider the four frame vectors \( \varphi_1 = [0.35 - 0.61]^\ast, \varphi_2 = [0.61 0.35]^\ast, \varphi_3 = [0.5 - 0.5]^\ast, \) and \( \varphi_4 = [0.5 0.5]^\ast \). The frame matrix associated with this frame is

\[
F = \begin{bmatrix}
0.35 & 0.61 & 0.5 & 0.5 \\
-0.61 & 0.35 & -0.5 & 0.5
\end{bmatrix}; \tag{25}
\]

we may check that \( F \) is indeed the frame matrix of a tight frame since \( FF^\ast = I_2 \).

We wish to construct an orthogonal frame matrix \( \tilde{F} \) such that \( F = P_\tilde{U} \tilde{F} \). In the proof of Theorem 3 for the case \( \dim \mathcal{H} < n \), we constructed an \( n \times n \) unitary matrix \( \tilde{F} \) using the SVD \( F = U \Sigma V^\ast \). Using this construction here, we obtain:

\[
U = \begin{bmatrix}
0.5 & -0.87 \\
-0.87 & -0.5
\end{bmatrix}, \quad \Sigma = \begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0
\end{bmatrix}, \quad V = \begin{bmatrix}
0.70 & 0 & 0.70 & 0 \\
0 & -0.70 & 0 & -0.70 \\
0.68 & -0.18 & -0.68 & 0.18 \\
-0.18 & -0.68 & 0.18 & 0.68
\end{bmatrix}. \tag{26}
\]

We now define the extended frame matrix \( \tilde{U} \) in accordance with the proof of Theorem 3. The first two columns of \( \tilde{U} \) are uniquely defined as the first two columns of \( U \) with zeroes appended. The remaining two columns are arbitrary, as long as the resulting \( \tilde{U} \) is unitary. A possible choice is:

\[
\tilde{U} = \begin{bmatrix}
0.5 & -0.87 & 0 & 0 \\
-0.87 & -0.5 & 0 & 0 \\
0 & 0 & 0.5 & -0.87 \\
0 & 0 & -0.87 & -0.5
\end{bmatrix}. \tag{27}
\]
Then

\[ \tilde{F} = \tilde{U}V^* = \begin{bmatrix} 
0.35 & 0.61 & 0.5 & 0.5 \\
-0.61 & 0.35 & -0.5 & 0.5 \\
0.35 & 0.61 & -0.5 & -0.5 \\
-0.61 & 0.35 & 0.5 & -0.5 
\end{bmatrix}. \]  

(28)

We may immediately verify that \( \tilde{F}^*\tilde{F} = I_4 \); i.e., \( \tilde{F} \) represents an orthonormal set of vectors.

Since the columns of \( F \) span a 2-dimensional Hilbert space \( \mathcal{U} = \mathcal{H} \), the projection onto this space is given by

\[ P_\mathcal{U} = \begin{bmatrix} 
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 
\end{bmatrix}, \]  

(29)

and indeed \( F = P_\mathcal{U}\tilde{F} \).

**Example 2.** We now consider an example in which \( \dim \mathcal{H} > n \). The construction of \( \tilde{F} \) is simpler than in the previous case because we do not have to extend \( \mathcal{H} \). Consider the three frame vectors \( \varphi_1 = \frac{1}{2}[1 \ 1 \ 1]^* \), \( \varphi_2 = \frac{1}{2}[-1 \ 1 \ 1]^* \), and \( \varphi_3 = \frac{1}{2}[\sqrt{2} \ 0 \ 0]^* \). The frame matrix associated with this frame is

\[ F = \frac{1}{2} \begin{bmatrix} 
1 & -1 & \sqrt{2} \\
1 & 1 & 0 \\
1 & 1 & 0 
\end{bmatrix}. \]  

(30)

In order to verify that \( F \) is indeed the frame matrix of a tight frame, we again determine the
SVD $F = U \Sigma V^*$, which yields

$$U = \begin{bmatrix}
0.58 & 0.82 & 0 \\
0.58 & -0.4 & 0.7 \\
0.58 & -0.4 & -0.7 \\
\end{bmatrix}, \quad \Sigma = \begin{bmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 0 \\
\end{bmatrix}, \quad V = \begin{bmatrix}
0.87 & 0 & 0.5 \\
0.29 & -0.82 & -0.5 \\
0.4 & 0.58 & -0.7 \\
\end{bmatrix}. \quad (31)$$

From Theorem 5 we conclude that $F$ is indeed the frame matrix of a tight frame since its nonzero singular values are all equal to 1; i.e., $F$ is a transjector. A basis for the subspace $U$ spanned by the columns of $F$ is the two vectors

$$u_1 = \begin{bmatrix}
0.58 \\
0.58 \\
0.58 \\
\end{bmatrix}^*, \quad u_2 = \begin{bmatrix}
0.82 \\
-0.4 \\
-0.4 \\
\end{bmatrix}^*. \quad (32)$$

Thus, $P_U$ is given by

$$P_U = \sum_{i=1}^{2} u_i u_i^T = \begin{bmatrix}
1 & 0 & 0 \\
0 & 0.5 & 0.5 \\
0 & 0.5 & 0.5 \\
\end{bmatrix}; \quad (33)$$

and indeed $FF^* = P_U$.

We now define an extended frame matrix $\tilde{F}$ such that $F = P_U \tilde{F}$ and $\tilde{F}^* \tilde{F} = I_3$. From the proof of Theorem 3 we have

$$\tilde{F} = U Z_3 V^* = UV^* = F + u_3 v_3^* = \begin{bmatrix}
0.5 & -0.5 & 0.7 \\
0.85 & 0.15 & -0.5 \\
0.15 & 0.85 & 0.5 \\
\end{bmatrix}, \quad (34)$$

where

$$u_3 = \begin{bmatrix}
0 & 0.7 & -0.7 \\
\end{bmatrix}^*, \quad v_3 = \begin{bmatrix}
0.5 & -0.5 & 0.7 \\
\end{bmatrix}^*. \quad (35)$$

Since $P_U u_3 v_3^* = 0$, we have immediately that $F = P_U \tilde{F}$.  

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5 Optimal Tight Frames

It is often of interest to construct a tight frame from a given set of vectors \( \{ \phi_i, 1 \leq i \leq n \} \). Different constructions have been proposed in the literature \([3, 8, 17]\); however, in the general case no optimality properties are known for these different constructions. Using the least-squares measurement (LSM) developed in the context of quantum detection \([28]\), we now propose a systematic method of constructing optimal tight frames from a given set of vectors.

Thus we seek to construct a tight frame of vectors \( \{ \varphi_i, 1 \leq i \leq n \} \) from a given set of vectors \( \{ \phi_i, 1 \leq i \leq n \} \) that span an \( r \)-dimensional space \( U \subseteq \mathcal{H} \). A reasonable approach is to find a set of vectors \( \varphi_i \in U \) that are “closest” to the vectors \( \phi_i \) in the least-squares sense. Thus we seek vectors \( \varphi_i \) that minimize the squared error \( E \), defined by

\[
E = \sum_{i=1}^{n} \langle e_i, e_i \rangle, \tag{36}
\]

where \( e_i \) denotes the \( i \)th error vector

\[
e_i = \phi_i - \varphi_i, \tag{37}
\]

subject to the constraint \([22]\).

We may wish to constrain the scaling \( \beta \) in \([22]\), e.g., we may seek a normalized tight frame with \( \beta = 1 \). The optimal frame in this case is derived in Section 5.1 and is referred to as the constrained least-squares frame (CLSF). Alternatively, we may choose the vectors \( \{ \varphi_i \} \) and \( \beta \) to satisfy \([22]\) and to minimize the squared error \( E \) of \([36]\). The optimal frame is then referred to as the unconstrained least-squares frame (ULSF), and is derived in Section 5.2.
5.1 Constrained least-squares frame

We first consider the problem of constructing a set of vectors \( \{\varphi_i, 1 \leq i \leq n\} \) that minimize \( E \) of (36), subject to the constraint

\[
\sum_{i=1}^{n} \varphi_i \varphi_i^* = \beta_0^2 P_U,
\]

(38)

where \( \beta_0^2 \) is specified. In the case of a normalized tight frame \( \beta_0^2 = 1 \).

If the vectors \( \phi_i \) are mutually orthogonal with \( \langle \phi_i, \phi_i \rangle = \beta_0^2 \), then the solution to (36) satisfying the constraint (38) is simply \( \varphi_i = \phi_i \), 1 \( \leq i \leq n \), which yields \( E = 0 \).

To derive the solution in the general case, denote by \( F \) and \( \Phi \) the \( k \times n \) matrices whose columns are the vectors \( \varphi_i \) and \( \phi_i \), respectively. The squared error \( E \) of (36)-(37) may then be expressed in terms of these matrices as

\[
E = \text{Tr} ((\Phi - F)^*(\Phi - F)) = \text{Tr} ((\Phi - F)(\Phi - F)^*).
\]

(39)

The constraint (22) may then be restated as

\[
FF^* = \beta_0^2 P_U.
\]

(40)

The least-squares problem of (39) seeks a frame matrix \( F \) that is “close” to the matrix \( \Phi \). If the two matrices are close, then we expect that the underlying linear transformations they represent will share similar properties. The SVD of \( \Phi \) specifies orthonormal bases for \( V \) and \( U \) such that the linear transformations \( \Phi \) and \( \Phi^* \) map one basis to the other with appropriate scale factors. Thus, to find an \( F \) close to \( \Phi \) we need to find a linear transformation \( F \) that performs a map similar to \( \Phi \). Employing the SVD \( \Phi = U\Sigma V^* \), we rewrite the squared error \( E \) of (39) as

\[
E = \text{Tr} ((\Phi - F)(\Phi - F)^*) = \text{Tr} (U^*(\Phi - F)(\Phi - F)^*U) = \sum_{i=1}^{k} \langle d_i, d_i \rangle,
\]

(41)
where

$$d_i = (\Phi - F)^*u_i. \quad (42)$$

The vectors \(\{u_i, 1 \leq i \leq r\}\) form an orthonormal basis for \(\mathcal{U}\). Therefore, the projection operator onto \(\mathcal{U}\) is given by

$$P_\mathcal{U} = \sum_{i=1}^{r} u_i u_i^*. \quad (43)$$

Essentially, we want to construct a map \(F^*\) such that the images of the maps defined by \(\Phi^*\) and \(F^*\) are as close as possible in the squared norm sense, subject to the constraint

$$FF^* = \beta_0^2 \sum_{i=1}^{r} u_i u_i^*. \quad (44)$$

The SVD of \(\Phi^*\) is given by \(\Phi^* = V\Sigma^*U^*\). Consequently,

$$\Phi^* u_i = \begin{cases} \sigma_i v_i, & 1 \leq i \leq r; \\ 0, & r + 1 \leq i \leq k, \end{cases} \quad (45)$$

where 0 denotes the zero vector. Denoting the image of \(u_i\) under \(F^*\) by \(a_i = F^*u_i\), for any choice of \(F\) satisfying the constraint (44) we have

$$\langle a_i, a_i \rangle = u_i^* FF^* u_i = \begin{cases} \beta_0^2, & 1 \leq i \leq r; \\ 0, & r + 1 \leq i \leq k, \end{cases} \quad (46)$$

and

$$\langle a_i, a_j \rangle = u_i^* FF^* u_j = 0, \quad i \neq j. \quad (47)$$

Thus the vectors \(a_i, 1 \leq i \leq r\), are mutually orthogonal with \(\langle a_i, a_i \rangle = \beta_0^2\) and \(a_i = 0, \quad m + 1 \leq
\( i \leq k \). Combining (45) and (46), we may express \( d_i \) as

\[
d_i = \begin{cases} 
\sigma_i v_i - a_i, & 1 \leq i \leq r; \\
0, & r + 1 \leq i \leq k.
\end{cases}
\] (48)

Our problem therefore reduces to finding a set of \( r \) orthogonal vectors \( a_i \) with norm \( \beta_0 \) that minimize \( E = \sum_{i=1}^{r} \langle d_i, d_i \rangle \), where \( d_i = \sigma_i v_i - a_i \). Since the vectors \( v_i \) are orthonormal, the minimizing vectors must be \( a_i = \beta_0 v_i, \ 1 \leq i \leq r \).

Thus the optimal frame matrix \( F \), denoted by \( \hat{F}_c \), satisfies

\[
\hat{F}_c^* u_i = \begin{cases} 
\beta_0 v_i, & 1 \leq i \leq r; \\
0, & r + 1 \leq i \leq k.
\end{cases}
\] (49)

Consequently

\[
\hat{F}_c = \beta_0 \sum_{i=1}^{r} u_i v_i^*.
\] (50)

We may express \( \hat{F}_c \) in matrix form as

\[
\hat{F}_c = \beta_0 U Z_r V^*,
\] (51)

where \( Z_r \) is defined by (1). The residual squared error is then

\[
E^{c}_{\text{min}} = \sum_{i=1}^{r} (\beta_0 - \sigma_i)^2 \langle v_i, v_i \rangle = \sum_{i=1}^{m} (\beta_0 - \sigma_i)^2.
\] (52)

Note that if the singular values \( \sigma_i \) are distinct, then the vectors \( u_i, \ 1 \leq i \leq r \) are unique (up to a phase factor \( e^{j\theta_i} \)). Given the vectors \( u_i \), the vectors \( v_i \) are uniquely determined, so the optimal frame vectors corresponding to \( \hat{F}_c \) are unique. If, on the other hand, there are repeated singular values, then the corresponding eigenvectors are not unique. Nonetheless, the choice of singular
vectors does not affect $\hat{F}_c$. Indeed, if the vectors corresponding to a repeated singular values are \{u_j\}, then \(\sum_j u_j u_j^*\) is a projection onto the corresponding eigenspace, and therefore is the same regardless of the choice of the vectors \{u_j\}. Thus

$$\sum_j u_j v_j^* = \frac{1}{\sigma} \sum_j u_j u_j^* \Phi,$$

(53)

independent of the choice of \{u_j\}, and the optimal frame is unique.

We may express $\hat{F}_c$ directly in terms of $\Phi$ as

$$\hat{F}_c = \beta_0 \Phi((\Phi^* \Phi)^{1/2})^\dagger,$$

(54)

where \((\cdot)^\dagger\) denotes the Moore-Penrose pseudo-inverse \[39\]. Indeed, \((\Phi^* \Phi)^{1/2})^\dagger = V((\Sigma^* \Sigma)^{1/2})^\dagger V^*\), where \(((\Sigma^* \Sigma)^{1/2})^\dagger\) is a diagonal matrix with diagonal elements \(1/\sigma_i\) for \(1 \leq i \leq r\) and 0 otherwise, so that $\Phi((\Phi^* \Phi)^{1/2})^\dagger = U Z_s V^*$.

Alternatively, $\hat{F}_c$ may be expressed as

$$\hat{F}_c = \beta_0 ((\Phi \Phi^*)^{1/2})^\dagger \Phi,$$

(55)

where \(((\Phi \Phi^*)^{1/2})^\dagger\) = \(U ((\Sigma \Sigma^*)^{1/2})^\dagger U^*\).

We note that the optimal frame vectors $\hat{\varphi}_i^c$ satisfy

$$\langle \hat{\varphi}_i^c, \phi_i \rangle = [\hat{F}_c^* \Phi]_{ii} = \beta_0 [\Phi^* \Phi]_{ii}^{1/2},$$

(56)

where \([\cdot]_{ii}\) denotes the \(ii\)th element of the matrix. This relation may be used to derive bounds on the inner products $\langle \hat{\varphi}_i^c, \phi_i \rangle$ in terms of the inner products $\langle \phi_i, \phi_j \rangle$; see \[37\].
5.1.1 Optimal orthogonal basis and the CLSF

In the previous section, we sought the $\beta_0$-scaled tight frame that minimizes the least-squares error. We may similarly seek the optimal orthogonal vectors with norm $\beta_0$ of the same form. We now explore the connection between the resulting optimal vectors both in the case of linearly independent vectors $\phi_i$ ($r = n$), and in the case of linearly dependent vectors ($r < n$).

**Linearly independent vectors:** If the vectors $\phi_i$ are linearly independent and consequently $\Phi$ has full column rank (i.e., $r = n$), then (54) reduces to

$$\hat{F}_c = \beta_0 \Phi (\Phi^* \Phi)^{-1/2}. \quad (57)$$

The optimal frame vectors $\hat{\varphi}_c^i$ are mutually orthogonal with equal norm $\beta_0$, since their Gram matrix is

$$\hat{F}_c^* \hat{F}_c = \beta_0^2 (\Phi^* \Phi)^{-1/2} \Phi^* \Phi (\Phi^* \Phi)^{-1/2} = \beta_0^2 I. \quad (58)$$

Thus, the optimal frame is in fact an optimal orthogonal basis for $\mathcal{U}$.

**Linearly dependent vectors:** If the vectors $\phi_i$ are linearly dependent, so that the matrix $\Phi$ does not have full column rank (i.e., $r < n$), then the $n$ frame vectors $\varphi_i^c$ cannot be mutually orthogonal since they span an $r$-dimensional subspace. We now try to gain some insight into the optimal frame vectors in this case. Our problem is to find a set of vectors that are as close as possible to the $n$ vectors $\phi_i$, which lie in an $r$-dimensional subspace $\mathcal{U}$. We now show that these vectors are the projections onto $\mathcal{U}$ of the set of norm-$\beta_0$ orthogonal vectors in $\mathcal{H}$ that are closest to the vectors $\phi_i$.

To see this, suppose we seek a set of orthogonal vectors $\tilde{\varphi}_i \in \mathcal{H}$ with $\langle \tilde{\varphi}_i, \tilde{\varphi}_i \rangle = \beta_0^2$ that are as close as possible to the vectors $\phi_i$. From Theorem 3 we have that

$$\sum_{i=1}^n \tilde{\varphi}_i \tilde{\varphi}_i^* = \beta_0^2 P_\mathcal{U}, \quad (59)$$

29
where \( \tilde{U} \supseteq U \) is the space spanned by the vectors \( \tilde{\varphi}_i \).

Since there are at most \( r \) orthogonal vectors in \( U \), imposing an orthogonality constraint forces the optimal orthogonal vectors \( \tilde{\varphi}_i \) to lie partly in the orthogonal complement \( U^\perp \). Each vector then has a component in \( U \), \( \tilde{\varphi}_U \), and a component in \( U^\perp \), \( \tilde{\varphi}_{U^\perp} \). Using (59), the component in \( U \) satisfies

\[
\sum_{i=1}^{n} \tilde{\varphi}_U^*(\tilde{\varphi}_U) = \sum_{i=1}^{n} P_U \tilde{\varphi}_i \tilde{\varphi}_i^* P_U = \beta_0^2 P_U P_U P_U = \beta_0^2 P_U,
\]

where the last equality follows from the fact that \( U \subseteq \tilde{U} \). Now we rewrite the error \( E \) of (36) as

\[
E = \sum_{i=1}^{n} \langle \phi_i - \tilde{\varphi}_U^i, \phi_i - \tilde{\varphi}_U^i \rangle
\]

\[
= \sum_{i=1}^{n} \left( \langle \phi_i - \tilde{\varphi}_U^i, \phi_i - \tilde{\varphi}_U^i \rangle + \langle \tilde{\varphi}_U^i, \tilde{\varphi}_U^i \rangle \right),
\]

since \( \langle \phi_i - \tilde{\varphi}_U^i, \tilde{\varphi}_U^i \rangle = 0 \). From (60) we have that

\[
\sum_{i=1}^{n} \langle \tilde{\varphi}_U^i, \tilde{\varphi}_U^i \rangle = \sum_{i=1}^{n} \langle \tilde{\varphi}_i, \tilde{\varphi}_i \rangle - \sum_{i=1}^{n} \langle \tilde{\varphi}_U^i, \tilde{\varphi}_U^i \rangle
\]

\[
= n \beta_0^2 - \text{Tr} \left( \sum_{i=1}^{n} \tilde{\varphi}_i^* \tilde{\varphi}_i^* \right)
\]

\[
= n \beta_0^2 - \text{Tr}(\beta_0^2 P_U) = (n - r) \beta_0^2,
\]

independent of the choice of vectors \( \tilde{\varphi}_i \). Thus, minimization of \( E \) is equivalent to minimization of

\[
E' = \sum_{i=1}^{n} \langle \phi_i - \tilde{\varphi}_U^i, \phi_i - \tilde{\varphi}_U^i \rangle.
\]

Furthermore, from (60) the vectors \( \tilde{\varphi}_U^i \) form a \( \beta_0 \)-scaled tight frame for \( U \).

We conclude that choosing a set of orthogonal vectors with equal norm \( \beta_0 \) that minimize \( E \) is equivalent to choosing an optimal \( \beta_0 \)-scaled tight frame for \( U \). The optimal orthogonal vectors
are not unique; however, their projections onto $U$ are unique and are just the optimal $\beta_0$-scaled tight frame vectors. We may choose the projections of the optimal orthogonal vectors onto $U^\perp$ arbitrarily, as long as the resulting $n$ vectors are orthogonal with norm $\beta_0$. A convenient choice is

$$\hat{F}_c = \beta_0 \sum_{i=1}^{n} u_i v_i.$$  \hspace{1cm} (64)

Indeed, Theorem 6 shows that the optimal orthogonal vectors are just a realization of the optimal frame vectors. This theorem guarantees that any $\beta_0$-scaled tight frame may be realized by a set of orthogonal vectors with norm $\beta_0$ in an extended space such that their projections onto the smaller space are the given frame vectors. Denoting by $\hat{\varphi}_i^c$ and $\hat{\varphi}_i^c$ the optimal frame vectors and orthogonal vectors, respectively, \[(13) \text{ asserts that} \]

$$\hat{\varphi}_i^c = P_U \hat{\varphi}_i^c.$$  \hspace{1cm} (65)

We summarize our results regarding the CLSF in the following theorem:

**Theorem 7 (Constrained least-squares frame (CLSF)).** Let $\{\phi_i\}$ be a set of $n$ vectors in a $k$-dimensional complex Hilbert space $\mathcal{H}$ that span an $r$-dimensional subspace $U \subseteq \mathcal{H}$. Let $\{\hat{\varphi}_i\}$ denote the optimal $n$ frame vectors that minimize the least-squares error defined by \[(38)-(39), \text{ subject to the constraint (38).} \text{ Let } \Phi = U \Sigma V^* \text{ be the rank-$r$ } k \times n \text{ matrix whose columns are the vectors } \phi_i, \text{ and let } \hat{F}_c \text{ be the } k \times n \text{ frame matrix whose columns are the vectors } \hat{\varphi}_i^c. \text{ Then the unique optimal } \hat{F}_c \text{ is given by}

$$\hat{F}_c = \beta_0 \sum_{i=1}^{r} u_i v_i^* = \beta_0 U Z_r V^* = \beta_0 \Phi (\Phi^* \Phi)^{1/2})^\dagger = \beta_0 ((\Phi^* \Phi)^{1/2})^\dagger \Phi,$$

where $u_i$ and $v_i$ denote the columns of $U$ and $V$ respectively and $Z_r$ is defined by \[(4). \]
The residual squared error is given by

\[ E_{\text{min}} = \sum_{i=1}^{r} (\beta_0 - \sigma_i)^2, \]

where \( \{\sigma_i, 1 \leq i \leq r\} \) are the nonzero singular values of \( \Phi \).

In addition,

1. If \( r = n \),
   (a) \( \hat{F}_c = \beta_0 \Phi (\Phi^* \Phi)^{-1/2} \);
   (b) \( \hat{F}_c^* \hat{F}_c = \beta_0^2 I_n \), and the corresponding frame vectors are orthogonal with norm \( \beta_0 \).

2. If \( r < n \),
   (a) \( \hat{F}_c \) may be realized by the \( \beta_0 \)-scaled optimal orthogonal frame matrix \( \hat{\tilde{F}}_c = \beta_0 \sum_{i=1}^{n} u_i v_i^* = \beta_0 U Z_n V^* \);
   (b) the action of the two optimal vector sets in the subspace \( \mathcal{U} \) is the same.

5.2 Unconstrained least-squares frame

We now consider the least-squares problem where the scaling of the frame is not constrained. Thus, we seek a set of vectors \( \{\varphi_i\} \) that minimize the squared error \( E \) of (36), subject to

\[ \sum_{i=1}^{n} \varphi_i \varphi_i^* = F F^* = \beta^2 P_U, \tag{66} \]

where \( F \) is the matrix of columns \( \varphi_i \), and \( \beta > 0 \).

The derivation of the solution to this minimization problem is very similar to the derivation of the CLSF of Section 5.1. Following the same steps, we can express \( E \) as

\[ E = \sum_{i=1}^{k} \langle d_i, d_i \rangle, \tag{67} \]
where $d_i = \sigma_i v_i - a_i$.

For any choice of $F$ satisfying the constraint (66) we have

$$\langle a_i, a_i \rangle = u_i^* F^* u_i = \begin{cases} \beta^2, & 1 \leq i \leq r; \\ 0, & r + 1 \leq i \leq k, \end{cases}$$

(68)

and

$$\langle a_i, a_j \rangle = u_i^* F^* u_j = 0, \ i \neq j.$$

(69)

Thus the vectors $a_i, 1 \leq i \leq r$, are mutually orthogonal with $\langle a_i, a_i \rangle = \beta^2$ and $a_i = 0, \ r+1 \leq i \leq k$.

Our problem therefore reduces to finding a set of $r$ orthogonal vectors $a_i$ with equal norm $\beta$ that minimize (67). Expressing $E$ as

$$E = \sum_{i=1}^{r} \left( \sigma_i^2 + \langle a_i, a_i \rangle - 2\sigma_i \Re \{ \langle a_i, v_i \rangle \} \right),$$

(70)

where $\Re \{ \cdot \}$ denotes the real part, we see that minimization of $E$ is equivalent to minimization of

$$E' = \sum_{i=1}^{r} \sigma_i \Re \{ \langle a_i, v_i \rangle \} = \beta^2 - 2\beta \sum_{i=1}^{r} \sigma_i \Re \{ \langle \tilde{a}_i, v_i \rangle \},$$

(71)

where $\tilde{a}_i = a_i / \beta$. To determine the optimal vectors $a_i$ we have to minimize $E'$ with respect to $\beta$ and $\tilde{a}_i$. Fixing $\tilde{a}_i$ and minimizing with respect to $\beta$, the optimal value of $\beta$ is given by

$$\hat{\beta} = \frac{1}{r} \sum_{i=1}^{r} \sigma_i \Re \{ \langle \tilde{a}_i, v_i \rangle \}.$$  

(72)

Substituting $\hat{\beta}$ back into (71), we get that the vectors $\tilde{a}_i$ are chosen to maximize

$$\left( \sum_{i=1}^{r} \sigma_i \Re \{ \langle \tilde{a}_i, v_i \rangle \} \right)^2,$$

(73)
subject to the constraint
\[ \langle \tilde{a}_i, \tilde{a}_j \rangle = \delta_{ij}. \]  
(74)

Since the vectors \( v_i \) are orthonormal, the minimizing vectors must be \( \tilde{a}_i = v_i, \ 1 \leq i \leq r \). Substituting into (72),
\[ \hat{\beta} = \frac{1}{r} \sum_{i=1}^{r} \sigma_i \Re \{ \langle v_i, v_i \rangle \} = \frac{1}{r} \sum_{i=1}^{r} \sigma_i \overset{\Delta}{=} \alpha, \]  
(75)

and \( a_i = \alpha v_i \).

Thus the optimal frame matrix \( F \), denoted by \( \hat{F}_u \), satisfies
\[ \hat{F}_u^* u_i = \begin{cases} \alpha v_i, & 1 \leq i \leq r; \\ 0, & r + 1 \leq i \leq k. \end{cases} \]  
(76)

Consequently
\[ \hat{F}_u = \alpha \sum_{i=1}^{r} u_i v_i^*. \]  
(77)

We may express \( \hat{F}_u \) in matrix form as
\[ \hat{F}_u = \alpha U Z_r V^* = \alpha \Phi((\Phi^* \Phi)^{1/2})^\dagger = \alpha((\Phi^*)^{1/2})^\dagger \Phi, \]  
(78)

where \( Z_r \) is defined by (1). The residual squared error is then
\[ E_{\text{min}}^u = \sum_{i=1}^{r} (\alpha - \sigma_i)^2 \langle v_i, v_i \rangle = \sum_{i=1}^{r} (\alpha - \sigma_i)^2. \]  
(79)

Recall that \( S = \Phi^* \Phi = V \Sigma^* \Sigma V^* \); thus \( \Tr(S) = \sum_{i=1}^{r} \sigma_i^2 \). Therefore,
\[ E_{\text{min}}^u = \Tr(S) - r \alpha^2. \]  
(80)

Note that as we expect \( E_{\text{min}}^u \leq E_{\text{min}}^c \), where \( E_{\text{min}}^u \) and \( E_{\text{min}}^c \) are given by (73) and (12) respectively,
with equality if and only if \( \beta_0 = \alpha \).

### 5.2.1 Optimal orthogonal basis and the ULSF

We now explore the connection between the least-squares orthogonal vectors with unconstrained norm and the ULSF.

**Linearly independent vectors:** If the vectors \( \phi_i \) are linearly independent and consequently \( \Phi \) has full column rank (i.e., \( r = n \)), then (78) reduces to

\[
\hat{F}_u = \alpha \Phi (\Phi^* \Phi)^{-1/2}.
\]

(81)

The optimal frame vectors \( \hat{\varphi}_i^u \) are mutually orthogonal with equal norm \( \alpha^2 \),

\[
\hat{F}_c^* \hat{F}_c = \alpha^2 (\Phi^* \Phi)^{-1/2} \Phi^* \Phi (\Phi^* \Phi)^{-1/2} = \alpha^2 I,
\]

and the optimal frame vectors are in fact the optimal orthogonal vectors.

**Linearly dependent vectors:** If the vectors \( \phi_i \) are linearly dependent, so that the matrix \( \Phi \) does not have full column rank (i.e., \( r < n \)), then the \( n \) frame vectors \( \varphi_i \) cannot be mutually orthogonal since they span an \( r \)-dimensional subspace. In analogy to the constrained case we now show that the optimal orthogonal vectors are related to the optimal frame vectors through a projection onto the subspace \( \mathcal{U} \), spanned by the vectors \( \phi_i \).

Suppose we seek a set of orthogonal vectors \( \tilde{\varphi}_i \in \mathcal{H} \) with equal norm that are as close as possible to the vectors \( \phi_i \). From Theorem 5 we have that

\[
\sum_{i=1}^{n} \tilde{\varphi}_i \tilde{\varphi}_i^* = \beta^2 P_{\tilde{U}},
\]

(83)

for some \( \beta > 0 \), where \( \tilde{U} \supset \mathcal{U} \) is the space spanned by the vectors \( \tilde{\varphi}_i \). Now, each vector \( \tilde{\varphi}_i \) has a
component in $\mathcal{U}$, $\varphi^H_i$, and a component in $\mathcal{U}^\perp$, $\varphi^\perp_i$. Using (83), the component in $\mathcal{U}$ satisfies
\[
\sum_{i=1}^n \varphi^H_i (\varphi^H_i)^* = \sum_{i=1}^n P_U \tilde{\varphi}_i \tilde{\varphi}_i^* P_U = \beta^2 P_U P_U P_U = \beta^2 P_U.
\]  (84)

From (84) we have that
\[
\sum_{i=1}^n \langle \varphi^\perp_i, \varphi^\perp_i \rangle = \sum_{i=1}^n \langle \tilde{\varphi}_i, \tilde{\varphi}_i \rangle - \sum_{i=1}^n \langle \varphi^H_i, \varphi^H_i \rangle = n\beta^2 - \text{Tr} \left( \sum_{i=1}^n \varphi^H_i (\varphi^H_i)^* \right) = n\beta^2 - \text{Tr}(\beta^2 P_U) = (n-r)\beta^2.
\]  (85)

Rewriting the error $E$ of (36) as in (61) and using (85), we conclude that minimization of $E$ is equivalent to minimizing
\[
E' = \sum_{i=1}^n \langle \varphi_i - \varphi^H_i, \varphi_i - \varphi^H_i \rangle + \beta^2 (n-r),
\]  (86)

where from (84) the vectors $\varphi^H_i$ form a $\beta$-scaled tight frame for $\mathcal{U}$.

Following the derivation of the ULSF, minimizing $E'$ is equivalent to minimizing
\[
E'' = r\beta^2 - 2\beta \sum_{i=1}^r \sigma_i \Re \{ \langle \tilde{a}_i, v_i \rangle \} + (n-r)\beta^2 = n\beta^2 - 2\beta \sum_{i=1}^r \sigma_i \Re \{ \langle \tilde{a}_i, v_i \rangle \},
\]  (87)

where $\tilde{a}_i = a_i/\beta$, $a_i = (\tilde{F}^H)^* u_i$, and $\tilde{F}^H$ is the matrix of columns $\varphi^H_i$. Fixing $\tilde{a}_i$ and minimizing with respect to $\beta$, the optimal value of $\beta$, denoted by $\tilde{\beta}$, is given by
\[
\tilde{\beta} = \frac{1}{n} \sum_{i=1}^r \sigma_i \Re \{ \langle \tilde{a}_i, v_i \rangle \}.
\]  (88)

Substituting $\tilde{\beta}$ back into (87), we get that the vectors $\tilde{a}_i$ are chosen to maximize (73) subject to
Thus, the minimizing vectors are $\tilde{a}_i = v_i$, $1 \leq i \leq r$. Substituting into (88) we have that

$$\hat{\beta} = \frac{1}{n} \sum_{i=1}^{r} \sigma_i \Re \{ \langle v_i, v_i \rangle \} = \frac{1}{n} \sum_{i=1}^{r} \sigma_i = \frac{r}{n} \alpha = \frac{\alpha}{\rho},$$

(89)

where $\alpha$ is defined in (75) and $\rho$ is the redundancy of the frame. Thus the optimal projections are the columns of $(1/\rho)\hat{F}_u$, where $\hat{F}_u$ is the frame matrix of the ULSF vectors.

We conclude that choosing a set of orthogonal vectors with unconstrained norm that minimize $E$ is equivalent to choosing an optimal unconstrained tight frame for $U$ and scaling these optimal frame vectors by $1/\rho$. The optimal unconstrained orthogonal vectors are not unique; however, their projections onto $U$ are unique and are proportional to the optimal unconstrained tight frame vectors. We may choose the projections of the optimal orthogonal vectors onto $U^\perp$ arbitrarily, as long as the resulting $n$ vectors are orthogonal with norm $\alpha/\rho$. A convenient choice is

$$\hat{F}_u = \frac{\alpha}{\rho} \sum_{i=1}^{n} u_i v_i^*.$$  

(90)

We summarize our results regarding the ULSF in the following theorem:

**Theorem 8 (Unconstrained least-squares frame (ULSF)).** Let $\{\phi_i\}$ be a set of $n$ vectors in a $k$-dimensional complex Hilbert space $\mathcal{H}$ that span an $r$-dimensional subspace $U \subseteq \mathcal{H}$. Let $\{\hat{\phi}_i^u\}$ denote the optimal $n$ frame vectors that minimize the least-squares error defined by (36)-(37), subject to the constraint (66). Let $\Phi = U\Sigma V^*$ be the rank-$m$ $k \times n$ matrix whose columns are the vectors $\phi_i$, and let $\hat{F}_u$ be the $k \times n$ frame matrix whose columns are the vectors $\hat{\phi}_i^u$. Then the unique optimal $\hat{F}_u$ is given by

$$\hat{F}_u = \alpha \sum_{i=1}^{r} u_i v_i^* = \alpha UZ_rV^* = \alpha \Phi((\Phi^*\Phi)^{1/2})^\dagger = \alpha((\Phi^*\Phi)^{1/2})^\dagger \Phi,$$

where $u_i$ and $v_i$ denote the columns of $U$ and $V$ respectively, $Z_r$ is defined in (4), $\alpha = \frac{1}{r} \sum_{i=1}^{r} \sigma_i$, and

$$\alpha = \frac{1}{r} \sum_{i=1}^{r} \sigma_i.$$
and \( \{\sigma_i, 1 \leq i \leq r\} \) are the nonzero singular values of \( \Phi \).

The residual squared error is given by

\[
E_{\min}^u = \sum_{i=1}^{r} (\alpha - \sigma_i)^2 = \text{Tr}(\Phi^*\Phi) - r\alpha^2.
\]

In addition,

1. If \( r = n \),
   
   (a) \( \hat{F}_u = \alpha \Phi (\Phi^*\Phi)^{-1/2} \);
   
   (b) \( \hat{F}_u^* \hat{F}_u = \alpha I_n \), and the corresponding frame vectors are orthogonal with norm \( \alpha \).

2. If \( r < n \), then \( (1/\rho) \hat{F}_u \) may be realized by the optimal orthogonal frame matrix \( \hat{F}_u = (\alpha/\rho) \sum_{i=1}^{n} u_i v_i^* \).

6 Connection with the Polar Decomposition

We now show that the ULSF and the CLSF are related to the polar decomposition of the matrix \( \Phi \).

Let \( \Phi \) denote an arbitrary \( k \times n \) matrix, where \( k \geq n \). Then \( \Phi \) has a polar decomposition\cite{40,41},

\[
\Phi = HY,
\]

where \( H \) is a \( k \times n \) partial isometry that satisfies \( H^*H = I_n \), and \( Y = (\Phi^*\Phi)^{1/2} \). The Hermitian factor \( Y \) is always unique; the partial isometry \( H \) is unique if and only if \( \Phi \) has full column rank.

If \( \Phi = U\Sigma V^* \) is the SVD of \( \Phi \), then a natural choice for \( H \) is

\[
H = UZ_n V^*,
\]

where \( U \) is the orthogonal matrix of left singular vectors, \( \Sigma \) is the diagonal matrix of singular values, \( V \) is the orthogonal matrix of right singular vectors, and \( Z_n \) is the \( n \times n \) partial isometry that satisfies \( Z_n^* Z_n = I_n \).
where $Z_n$ is given by (16). If $r = n$, then this choice of $H$ is unique. Otherwise $H$ is not unique; however, its projection onto the column space $\mathcal{U}$ of $\Phi$ is unique and is given by [22]

$$H_{\mathcal{U}} = P_{\mathcal{U}}H = UZ_rV^* = \Phi((\Phi^*\Phi)^{1/2})^\dagger,$$

(93)

where $Z_r$ is given by (1).

Comparing (93) with (51) and (78), we conclude that the ULSF and CLSF are proportional to the (unique) projection onto $\mathcal{U}$ of the partial isometry $H$ in a polar decomposition of $\Phi$. Thus, the ULSF and CLSF can be computed very efficiently by use of the many known efficient algorithms for computing the polar decomposition (see e.g., [39, 43, 40, 44]).

Recently the truncated polar decomposition (TPD), a variation on the polar decomposition, has been introduced [45] and has proved to be useful for various estimation and detection problems. As we now show, the columns of the TPD of a matrix $\Phi$ are just the closest normalized frame vectors to the columns $\phi_i$ of $\Phi$.

Let $\Phi = U\Sigma V^*$ denote an arbitrary $k \times n$ matrix with rank $r$. Then the order-$p$ TPD of $\Phi$ is the factorization

$$P_{\mathcal{U}_p}\Phi = [UZ_pV^*][V\Sigma^*Z_pV^*] = \tilde{H}\tilde{Y},$$

(94)

where $P_{\mathcal{U}_p}$ is the orthogonal projection onto the space spanned by the first $p$ singular vectors $u_i$ of $\Phi$. From (94) it follows that the left-hand matrix in the order-$r$ TPD of $\Phi$ is just the optimal normalized frame matrix $\hat{F}_c$. Similarly, the left-hand matrix in the order-$p$ TPD of $\Phi$, with $p < r$, is the optimal normalized tight frame matrix corresponding to the vectors $P_{\mathcal{U}_p}\phi_i$.

Since the CLSF and ULSF are related to the polar decomposition of $\Phi$, properties of these optimal frames can be deduced from properties of the polar decomposition (see e.g., [40, 41, 43, 46]). For example, the CLSF or ULSF corresponding to two vector sets $\{\phi_i\}$ and $\{\psi_i\}$ are the same if and only if the corresponding frame matrices satisfy $\Phi\Psi^* = ||\Phi||\Psi|$, where $|X| = X^*X$ [16].
7 Comparison with Other Proposed Frame Constructions

We now compare our results with previously proposed frame constructions.

The most popular frame construction from a given set of vectors is the canonical frame. Given a set of vectors \( \{\phi_i, 1 \leq i \leq n\} \) the canonical frame associated with these vectors is the frame corresponding to the frame matrix \( F = \Phi((\Phi^*\Phi)^{1/2})^\dagger \). (95)

The canonical frame has many desirable properties. Its construction is relatively simple; it can be determined directly from the given vectors; and if the vectors \( \phi_i \) are linearly independent, then it produces an orthonormal basis for \( U \). This construction was first proposed in the context of wavelets in [24], and plays an important role in wavelet theory [25, 26, 27]. However, no general optimality properties are known for the canonical frame.

Comparing (95) with (54), we see immediately that the canonical frame vectors are just the normalized tight frame vectors that are closest in a least-squares sense to the vectors \( \{\phi_i\} \). Furthermore, the \( \beta_0 \)-scaled tight frame vectors that are closest to the vectors \( \{\phi_i\} \) are the canonical frame vectors scaled by \( \beta_0 \).

From Theorem 8, it follows that the canonical frame vectors are the tight frame vectors that minimize the least-squares error only if \( \alpha = 1 \), i.e., only if \( \sum_{i=1}^r \sigma_i = r \). Otherwise, the canonical frame is no longer the optimal tight frame in a least-squares sense. However, if we simply scale each of the canonical frame vectors by \( \alpha \), then the resulting frame minimizes the least-squares error among all possible tight frames.
We summarize our results regarding canonical frames in the following theorem:

**Theorem 9 (Canonical frames).** Let \( \{\phi_i\} \) be a set of \( n \) vectors in a \( k \)-dimensional complex Hilbert space \( \mathcal{H} \) that span an \( r \)-dimensional subspace \( U \subseteq \mathcal{H} \). Let \( \Phi = U \Sigma V^* \) be the rank-\( r \) \( k \times n \) matrix whose columns are the vectors \( \phi_i \). Let \( u_i \) and \( v_i \) denote the columns of the unitary matrices \( U \) and \( V \) respectively, let \( \{\sigma_i, 1 \leq i \leq r\} \) denote the nonzero singular values of \( \Phi \), and let \( Z_r \) be defined as in (1). Let \( \{\varphi_i\} \) be the \( n \) canonical frame vectors associated with the vectors \( \phi_i \), and let \( F \) denote the matrix of columns \( \varphi_i \). Then

\[
F = U Z_r V^* = \Phi ((\Phi^* \Phi)^{1/2})^{1/2} = ((\Phi \Phi^*)^{1/2})^{1/2} \Phi.
\]

In addition,

1. If \( r = n \),
   
   (a) the canonical frame vectors form an orthonormal basis for \( U \);
   
   (b) the canonical frame vectors are the closest orthonormal vectors to the vectors \( \{\phi_i\} \), in a least-squares sense;
   
   (c) if \( \sum_{i=1}^r \sigma_i = r \), then the canonical frame vectors are the closest orthogonal vectors with equal norm to the vectors \( \{\phi_i\} \), in a least-squares sense;
   
   (d) define the scaled canonical frame vectors \( \varphi'_i = \beta \varphi_i \). Then
      
      i. the scaled canonical frame vectors are the closest orthogonal vectors with norm \( \beta \) to the vectors \( \{\phi_i\} \), in a least-squares sense;
        
      ii. if \( \beta = (1/r) \sum_{i=1}^r \sigma_i \), then the scaled canonical frame vectors are the closest orthogonal vectors with equal norm to the vectors \( \{\phi_i\} \), in a least-squares sense.

2. If \( r < n \),
   
   (a) the canonical frame vectors form a tight frame for \( U \);
(b) the canonical frame vectors are the closest normalized tight frame vectors to the vectors 
\{\phi_i\}, in a least-squares sense;

(c) if \(\sum_{i=1}^{r} \sigma_i = r\), then the canonical frame vectors are the closest tight frame vectors to the vectors \{\phi_i\}, in a least-squares sense;

(d) Define the scaled canonical frame vectors \(\varphi'_i = \beta \mu_i\). Then

i. the scaled canonical frame vectors are the closest \(\beta\)-scaled tight frame vectors to the vectors \{\phi_i\}, in a least-squares sense.

ii. if \(\beta = (1/r) \sum_{i=1}^{r} \sigma_i\), then the scaled canonical frame vectors are the closest tight frame vectors to the vectors \{\phi_i\}, in a least-squares sense.

8 Optimal Frames For Geometrically Uniform Vector Sets

An important issue in constructing frames from a given set of vectors, is to what extent the frames inherit the properties of the original vector set. In this section we consider the case in which the given vectors have a strong symmetry property, called geometric uniformity \(^{23}\). Under these conditions we can show that the optimal frame has the same symmetries as the original vector set.

For simplicity, we consider only the optimal normalized tight frame, which from Theorem \(^9\) coincides with the canonical frame. Since the canonical frame vectors are proportional to the vectors constituting the CLSF and the ULSF, the results extend in a straightforward manner to these more general constructions.

A set of vectors \(S = \{\phi_i, 1 \leq i \leq n\}\) is geometrically uniform (GU) if every vector in the set has the form \(\phi_i = U_i \phi\), where \(\phi\) is an arbitrary vector and the matrices \(\{U_i, 1 \leq i \leq n\}\) are unitary and form an abelian group \(\mathcal{G}\).

If the vectors \(\phi_i\) are GU, then every row (or column) of the Gram matrix \(S = \{\langle \phi_i, \phi_j \rangle\}\) is a

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\(^{23}\)That is, \(\mathcal{G}\) contains the identity matrix \(I\); if \(\mathcal{G}\) contains \(U_i\), then it also contains its inverse \(U_i^{-1}\); the product \(U_iU_j\) of any two elements of \(\mathcal{G}\) is in \(\mathcal{G}\); and \(U_iU_j = U_jU_i\) for any two elements in \(\mathcal{G}\).
permutation of the first row (or column) \[28\]: such a matrix will be called a permuted matrix. A set of vectors satisfying \[\langle \phi_i, \phi_j \rangle = \langle \phi_j, \phi_i \rangle \] for all \(i, j\) (as is the case e.g., for real vector sets) is GU if and only if the corresponding Gram matrix is a permuted matrix \[42\].

The canonical frame vectors corresponding to a GU vector set are conveniently characterized in terms of a Fourier matrix defined on an additive group \(G\) isomorphic \[47\] to \(G\). Specifically, it is well known (see e.g., \[47\]) that every finite abelian group \(G\) is isomorphic to a direct product \(G\) of a finite number of cyclic groups: \(G \cong G = \mathbb{Z}_{n_1} \times \cdots \times \mathbb{Z}_{n_p}\), where \(\mathbb{Z}_{n_t}\) is the cyclic additive group of integers modulo \(n_t\), and \(n = \prod_t n_t\). Thus every element \(U_i \in G\) can be associated with an element \(g \in G\) of the form \(g = (g_1, g_2, \ldots, g_p)\), where \(g_t \in \mathbb{Z}_{n_t}\); this correspondence is denoted by \(U_i \leftrightarrow g\).

Each vector \(\phi_i = U_i \phi\) is then denoted as \(\phi(g)\), where \(U_i \leftrightarrow g\).

The Fourier transform (FT) of a complex-valued function \(\varphi : G \rightarrow \mathbb{C}\) defined on \(G = \mathbb{Z}_{n_1} \times \cdots \times \mathbb{Z}_{n_p}\) is the complex-valued function \(\hat{\varphi} : G \rightarrow \mathbb{C}\) defined by

\[
\hat{\varphi}(h) = \frac{1}{\sqrt{n}} \sum_{g \in G} \langle h, g \rangle \varphi(g),
\]

(96)

where the Fourier kernel \(\langle h, g \rangle\) is

\[
\langle h, g \rangle = \prod_{t=1}^{p} e^{-2\pi i h_t g_t / n_t}.
\]

(97)

Here \(h_t\) and \(g_t\) are the \(k\)th components of \(h\) and \(g\) respectively, and the product \(h_t g_t\) is taken as an ordinary integer modulo \(n_t\).

The FT matrix over \(G\) is defined as the \(n \times n\) matrix \(F = \{\frac{1}{\sqrt{n}} \langle h, g \rangle, h, g \in G\}\). The FT of a column vector \(\varphi = \{\varphi(g), g \in G\}\) is then the column vector \(\hat{\varphi} = \{\hat{\varphi}(h), h \in G\}\) given by \(\hat{\varphi} = F \varphi\).

\footnote{Two groups \(G\) and \(G'\) are isomorphic, denoted by \(G \cong G'\), if there is a bijection (one-to-one and onto map) \(\varphi : G \rightarrow G'\) which satisfies \(\varphi(xy) = \varphi(x)\varphi(y)\) for all \(x, y \in G\) \[47\].}
Since $F$ is unitary, we obtain the inverse FT formula

$$\varphi = F^* \hat{\varphi} = \left\{ \frac{1}{\sqrt{n}} \sum_{h \in G} \langle h, g \rangle^* \hat{\varphi}(h), g \in G \right\}. \quad (98)$$

Following the development in [28], we can now obtain the following result:

**Theorem 10 (Least-squares normalized tight frames for GU vector sets).** Let $S = \{\phi_i = U_i \phi, U_i \in G\}$, be a geometrically uniform vector set generated by a finite abelian group $G$ of unitary matrices, where $\phi$ is an arbitrary vector, and let $\Phi$ be the matrix of columns $\phi_i$. Let $G$ be an additive abelian group isomorphic to $G$, let $\{\phi(g), g \in G\}$ be the elements of $S$ under this isomorphism, and let $F$ be the Fourier transform matrix over $G$. Then the normalized tight frame that is closest in the least-squares sense to $\Phi$ is given by the frame matrix

$$F = \Phi \Sigma^\dagger F^* = \sum_{h \in G} u(h) F^*(h),$$

where

1. $\Sigma^\dagger$ is the diagonal matrix whose diagonal elements are $\sigma(h)^{-1}$ when $\sigma(h) \neq 0$ and 0 otherwise,

2. $\{\sigma(h) = n^{1/4} \sqrt{s(h)}, h \in G\}$ are the singular values of $\Phi$,

3. $\{s(h), h \in G\}$ is the Fourier transform of the inner-product sequence $\{\langle \phi(0), \phi(g) \rangle, g \in G\}$;

4. $u(h) = \hat{\phi}(h)/\sigma(h)$ when $\sigma(h) \neq 0$ and 0 otherwise,

5. $\{\hat{\phi}(h), h \in G\}$ is the Fourier transform of $\{\phi(g), g \in G\}$;

6. $F^*(h)$ is the $h$th row of $F^*$.

Finally, the frame matrix $F$ has the same symmetries as $\Phi$. 

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8.1 Example of a GU vector set

We now consider an example demonstrating the ideas of the previous section. (The same example was given in [28].) Further examples and applications of GU vector sets can be found in [28].

Consider the group $G$ of $n = 4$ unitary matrices $U_i$, where

$$U_1 = I_4, \quad U_2 = \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}, \quad U_3 = \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}, \quad U_4 = U_2U_3. \quad (99)$$

Let the GU vector set be $S = \{\phi_i = U_i\phi, \ 1 \leq i \leq 4\}$, where $\phi = \frac{1}{2}[1 \ 1 \ 1 \ 1]^*$. Then $\Phi$ is

$$\Phi = \frac{1}{2} \begin{bmatrix} 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix}, \quad (100)$$

and the Gram matrix $S$ is given by

$$S = \frac{1}{2} \begin{bmatrix} 2 & -1 & -1 & 0 \\ -1 & 2 & 0 & -1 \\ -1 & 0 & 2 & -1 \\ 0 & -1 & -1 & 2 \end{bmatrix}. \quad (101)$$

Note that the sum of the vectors $\phi_i$ is 0, so the vector set is linearly dependent.

In this case $G$ is isomorphic to $G = \mathbb{Z}_2 \times \mathbb{Z}_2$, i.e., $G = \{(0,0), (0,1), (1,0), (1,1)\}$. The multipli-
cation table of the group $G$ is

|     | $U_1$ | $U_2$ | $U_3$ | $U_4$ |
|-----|------|------|------|------|
| $U_1$ | $U_1$ | $U_2$ | $U_3$ | $U_4$ |
| $U_2$ | $U_2$ | $U_1$ | $U_4$ | $U_3$ |
| $U_3$ | $U_3$ | $U_4$ | $U_1$ | $U_2$ |
| $U_4$ | $U_4$ | $U_3$ | $U_2$ | $U_1$ |

If we define the correspondence

$$U_1 \leftrightarrow (0, 0), \ U_2 \leftrightarrow (0, 1), \ U_3 \leftrightarrow (1, 0), \ U_4 \leftrightarrow (1, 1),$$

(103)

then this table becomes the addition table of $G = \mathbb{Z}_2 \times \mathbb{Z}_2$:

|     | $(0, 0)$ | $(0, 1)$ | $(1, 0)$ | $(1, 1)$ |
|-----|----------|----------|----------|----------|
| $(0, 0)$ | $(0, 0)$ | $(0, 1)$ | $(1, 0)$ | $(1, 1)$ |
| $(0, 1)$ | $(0, 1)$ | $(0, 0)$ | $(1, 1)$ | $(1, 0)$ |
| $(1, 0)$ | $(1, 0)$ | $(1, 1)$ | $(0, 0)$ | $(0, 1)$ |
| $(1, 1)$ | $(1, 1)$ | $(1, 0)$ | $(0, 1)$ | $(0, 0)$ |

(104)

Only the way in which the elements are labeled distinguishes the table of (104) from the table of (102); thus $G$ is isomorphic to $G$. Comparing (102) and (104) with (101), we see that the tables and the matrix $S$ have the same symmetries.

Over $G = \mathbb{Z}_2 \times \mathbb{Z}_2$, the Fourier matrix $\mathcal{F}$ is the Hadamard matrix

$$\mathcal{F} = \frac{1}{2} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix}.$$ 

(105)
Using the equations of the theorem, we may find the canonical frame:

\[
F = \frac{1}{2\sqrt{2}} \begin{bmatrix}
1 & -1 & -1 & 1 \\
\sqrt{2} & \sqrt{2} & -\sqrt{2} & -\sqrt{2} \\
\sqrt{2} & -\sqrt{2} & \sqrt{2} & -\sqrt{2} \\
1 & -1 & -1 & 1
\end{bmatrix}.
\]

(106)

We verify that the columns \(\varphi_i\) of \(F\) may be expressed as \(\varphi_i = U_i \varphi_1, 1 \leq i \leq 4\), where \(\varphi_1 = \frac{1}{2\sqrt{2}}[1 \sqrt{2} \sqrt{2} 1]^*\). Thus the frame vectors \(\varphi_i\) also form a GU set generated by \(G\).

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