

A GAP FOR THE MAXIMUM NUMBER OF MUTUALLY UNBIASED BASES

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ABSTRACT. A collection of pairwise mutually unbiased bases (in short: MUB) in $d > 1$ dimensions may consist of at most $d + 1$ bases. Such “complete” collections are known to exist in \mathbb{C}^d when d is a power of a prime. However, in general, little is known about the maximum number $N(d)$ of bases that a collection of MUB in \mathbb{C}^d can have.

In this work it is proved that a collection of d MUB in \mathbb{C}^d can always be completed. Hence $N(d) \neq d$, and when $d > 1$ we have a dichotomy: *either* $N(d) = d + 1$ (so that there exists a complete collection of MUB) *or* $N(d) \leq d - 1$. In the course of the proof an interesting new characterization is given for a linear subspace of $M_d(\mathbb{C})$ to be a subalgebra.

1. INTRODUCTION

Two orthonormal bases $\mathcal{E} = (\mathbf{e}_1, \dots, \mathbf{e}_d)$ and $\mathcal{F} = (\mathbf{f}_1, \dots, \mathbf{f}_d)$ in \mathbb{C}^d such that

$$(1.1) \quad |\langle \mathbf{e}_k, \mathbf{f}_j \rangle| = \text{constant} = \frac{1}{\sqrt{d}}$$

for all $k, j = 1, \dots, d$, are said to be **mutually unbiased**. A famous question regarding mutually unbiased bases (MUB) is the following: in a d -dimensional complex space, at most how many orthonormal bases can be given so that any two of them are mutually unbiased?

The motivation for the question comes from quantum information theory. MUB are useful in quantum state tomography [1], and the known quantum cryptographic protocols also rely on MUB; see for example [2].

Simple arguments show that the maximum number $N(d)$ of orthonormal bases in a collection of MUB satisfies the bound $N(d) \leq d + 1$ for every $d > 1$. A collection of $d + 1$ MUB is usually referred as a **complete collection**. When the dimension $d = p^\alpha$ is a power of a prime, such complete collections can be constructed [3, 4]. However, apart from this case, at the moment there is no dimension $d > 1$ in which the value of $N(d)$ would be known. So already in dimension six the problem is open. Nevertheless, numerical and other evidence [5, 6] suggest that $N(6) = 3$, which is much less than 7 (which we would need for a complete collection).

It seems that the problem of complete collections of MUB is deeply related to that of finite projective planes (or equivalently: to complete collections of mutually orthogonal Latin squares); see for example the construction [7] and the overview

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[8]. However, it has not been proved that either of the two — namely, the existence of a finite projective plane of order d and the existence of a complete collection of MUB in \mathbb{C}^d — would imply the other.

In this respect, the result of the present work can be considered as one more indication of the connection between the two questions. Here it will be proved that having a collection of d MUB in \mathbb{C}^d , one can always find and add one more basis with which it becomes a complete collection. In general, if a collection is “missing” two bases, it cannot always be completed and the first example for this occurs in $d = 4$ dimensions; see [9]. This is similar to the following. A collection of mutually orthogonal Latin squares “missing” only one element to be complete can be indeed completed.¹ In general, a collection of mutually orthogonal $n \times n$ Latin squares “missing” two elements cannot always be completed, and the smallest value² (and by [14] in fact the *only* value) of n for which such an incomplete collection can be given is $n = 4$.

One may have a look at the problem of MUB from several different points of view. One might consider looking at Lie algebra theory [15]. The original problem, which is formulated in a complex space, may also be turned into a real convex geometrical question and hence may be investigated with tools of convex geometry [16]. Often questions about MUB are rephrased in terms of complex Hadamard matrices; see for example [17]. However, for the author of this work, the most natural point of view is that of operator algebras (or, being in finite dimensions, perhaps it is better to say matrix algebras).

There is a natural way to associate a maximal abelian $*$ -subalgebra (in short, a MASA) to an orthonormal basis (ONB). In the context of matrix algebras, we consider a system of MASAs instead of a system of bases. Mutual unbiasedness is then expressed as a natural orthogonality relation (sometimes also called “quasi-orthogonality” or “complementarity of subalgebras”). In fact, in the study of matrix algebras one considers systems of orthogonal subalgebras *in general* (that is, systems consisting of all kind of subalgebras, not only maximal abelian ones). For the topic of orthogonal subalgebras and its relation to mutual unbiasedness, see for example [18, 19, 21, 20, 22] and [23]. Note that apart from the finite dimensional case, orthogonal subalgebras were also considered in the context of type II_1 von Neumann algebras; see [24].

Suppose $\mathcal{A}_1, \dots, \mathcal{A}_d, \mathcal{A}_{d+1}$ is a collection of orthogonal MASAs in $M_d(\mathbb{C})$. Then \mathcal{A}_{d+1} must be the orthogonal complement of $V := \sum_{k=1}^d (\mathcal{A}_k \cap \{\mathbb{1}\}^\perp)$. So if we are only given d orthogonal MASAs, then only at one place can we possibly find a MASA which is orthogonal to all of them: at the orthogonal complement of V . All we need to show is that this subspace of $M_d(\mathbb{C})$, which is *a priori* not even an algebra, is in fact a MASA. This will be done by first working out an interesting new characterization for a linear subspace of $M_d(\mathbb{C})$ to be a subalgebra.

¹This is well-known to experts of the field [10], but it is difficult to give a good reference. One may say that it is a subcase of [11, Theorem 4.3], but it is somewhat misleading, as the proof of this much stronger statement is difficult, whereas what we need is almost a triviality; e.g. in the textbook [12] it is given as an exercise.

²It is evident that for $n = 1, 2, 3$ there can be no such example. For $n = 4$ finding such an example simply means finding a “bachelor” 4×4 Latin square, i.e. one that has no orthogonal mate. The existence of bachelor Latin squares of many different sizes was already known to Euler, and in [13] it is proved that for any $n \geq 4$ there exists a bachelor Latin square.

Can we find a (closed “elementary”) expression giving the “missing basis” in terms of the others? It is clear where the “missing” MASA is, but to find the corresponding *basis* we would need to diagonalize the matrices appearing in our MASA. This might require finding the roots of certain characteristic polynomials. So note that it might well be that in general in dimensions $d \geq 5$ there is no (closed “elementary”) expression giving the missing basis.

2. PRELIMINARIES

Let $\mathcal{E} = (\mathbf{e}_1, \dots, \mathbf{e}_d)$ be an ONB in \mathbb{C}^d , and denote the ortho-projection onto the one-dimensional subspace $\mathbb{C}\mathbf{e}_j$ by $P_{\mathbf{e}_j}$ for each $j = 1, \dots, d$. Then we may consider

$$(2.1) \quad \mathcal{A}_{\mathcal{E}} = \text{Span}\{P_{\mathbf{e}_j} \mid j = 1, \dots, d\},$$

that is, the subspace of $M_d(\mathbb{C})$ spanned linearly by the ortho-projections $P_{\mathbf{e}_j}$ ($j = 1, \dots, d$). It is a MASA, and actually, if $\mathcal{A} \subset M_d(\mathbb{C})$ is a MASA, then there exists an ONB \mathcal{E} such that $\mathcal{A} = \mathcal{A}_{\mathcal{E}}$.

There is a natural scalar product on $M_d(\mathbb{C})$, the so-called *Hilbert-Schmidt* scalar product, defined by the formula

$$(2.2) \quad \langle A, B \rangle = \text{Tr}(A^*B) \quad (A, B \in M_d(\mathbb{C})).$$

In this sense, if $\mathcal{A} \subset M_d(\mathbb{C})$ is a given linear subspace, one can consider the ortho-projection $E_{\mathcal{A}}$ onto \mathcal{A} . When \mathcal{A} is actually a $*$ -subalgebra containing $\mathbb{1} \in M_d(\mathbb{C})$, then $E_{\mathcal{A}}$ is nothing else than the so-called *trace-preserving conditional expectation* onto \mathcal{A} . If more in particular $\mathcal{A} = \mathcal{A}_{\mathcal{E}}$ is the MASA associated to the ONB \mathcal{E} , then an easy check shows that

$$(2.3) \quad E_{\mathcal{A}_{\mathcal{E}}}(X) = \sum_{k=1}^d P_{\mathbf{e}_k} X P_{\mathbf{e}_k}$$

for all $X \in M_d(\mathbb{C})$.

Two MASAs $\mathcal{A}, \mathcal{B} \subset M_d(\mathbb{C})$, as subspaces, cannot be orthogonal, since $\mathcal{A} \cap \mathcal{B} \neq \{0\}$ as $\mathbb{1} \in \mathcal{A} \cap \mathcal{B}$. At most, the subspaces $\mathcal{A} \cap \{\mathbb{1}\}^{\perp}$ and $\mathcal{B} \cap \{\mathbb{1}\}^{\perp}$ can be orthogonal, in which case we say that \mathcal{A} and \mathcal{B} are **orthogonal subalgebras**. A direct consequence of the definitions of the Hilbert-Schmidt scalar product and of subalgebra orthogonality is that \mathcal{A} and \mathcal{B} are orthogonal subalgebras of $M_d(\mathbb{C})$ if and only if for all $A \in \mathcal{A}$ and $B \in \mathcal{B}$,

$$(2.4) \quad \tau(AB) = \tau(A)\tau(B),$$

where $\tau = \frac{1}{d}\text{Tr}$ is the normalized trace.

As is well-known — but in any case it can be obtained by simply substituting $A := P_{\mathbf{e}_k}$ and $B := P_{\mathbf{f}_j}$ into (2.4) — two MASAs $\mathcal{A}_{\mathcal{E}}$ and $\mathcal{A}_{\mathcal{F}}$ in $M_d(\mathbb{C})$ are orthogonal if and only if \mathcal{E} and \mathcal{F} are mutually unbiased. So the problem of finding a certain number of MUB is equivalent to finding the same number of orthogonal MASAs.

The dimension of $\mathcal{A} \cap \{\mathbb{1}\}^{\perp}$ is $\dim(\mathcal{A}) - 1 = d - 1$ for a MASA \mathcal{A} , whereas the dimension of $M_d(\mathbb{C}) \cap \{\mathbb{1}\}^{\perp}$ is $d^2 - 1$. However, if $d > 1$, then in a $(d^2 - 1)$ -dimensional space there can be at most

$$(2.5) \quad \frac{d^2 - 1}{d - 1} = d + 1$$

pairwise orthogonal $(d - 1)$ -dimensional subspaces. So when $d > 1$, a collection of orthogonal MASAs can have at most $d + 1$ elements; this is one of the ways one can obtain the well-known upper bound on $N(d)$.

We shall finish this section by recalling an important fact about orthonormal bases in $M_d(\mathbb{C})$. Its proof can be found for example in [25], but one could also have a look at [26, Proposition 1], which is a stronger generalization. However, for self-containment let us now see the statement together with its proof.

Lemma 2.1. *Let A_1, \dots, A_{d^2} be an ONB in $M_d(\mathbb{C})$. Then*

$$\sum_{k=1}^{d^2} A_k^* X A_k = \text{Tr}(X) \mathbb{1}$$

for all $X \in M_d(\mathbb{C})$.

Proof. Let B_1, \dots, B_{d^2} be another ONB in $M_d(\mathbb{C})$. Then there exist complex coefficients $\lambda_{k,j}$ ($k, j = 1, \dots, d^2$) such that $B_k = \sum_j \lambda_{k,j} A_j$. Since a linear map that takes an ONB into an ONB must be unitary, we have that $\sum_{k=1}^{d^2} \overline{\lambda_{k,j}} \lambda_{k,l} = \delta_{j,l}$. Hence

$$(2.6) \quad \sum_{k=1}^{d^2} B_k^* X B_k = \sum_{k,j,l=1}^{d^2} (\lambda_{k,j} A_j)^* X (\lambda_{k,l} A_k) = \sum_{k,j,l=1}^{d^2} \overline{\lambda_{k,j}} \lambda_{k,l} A_j^* X A_l = \sum_{j=1}^{d^2} A_j^* X A_j,$$

showing that the sum appearing in the statement is independent of the chosen ONB. Thus the formula can be verified by an elementary check using the ONB consisting of “matrix units”. \square

Note that the same argument, together with formula (2.3), shows that if $\mathcal{A} \subset M_d(\mathbb{C})$ is a MASA, then for any ONB A_1, \dots, A_d in \mathcal{A} we have that

$$(2.7) \quad E_{\mathcal{A}}(X) = \sum_k A_k^* X A_k$$

for all $X \in M_d(\mathbb{C})$.

3. THE “MISSING” BASIS FOUND

Suppose we are given a collection of d MUB in \mathbb{C}^d . As was explained, this gives us d pairwise orthogonal MASAs in $M_d(\mathbb{C})$; let us denote them by $\mathcal{A}_1, \dots, \mathcal{A}_d$.

The subspaces $\mathcal{A}_k \cap \{\mathbb{1}\}^\perp$ ($k = 1, \dots, d$) are $(d - 1)$ -dimensional, orthogonal subspaces. Hence $V := \sum_{k=1}^d (\mathcal{A}_k \cap \{\mathbb{1}\}^\perp)$ is $(d^2 - d)$ -dimensional, and V^\perp is a d -dimensional subspace in $M_d(\mathbb{C})$. Our aim is to prove that $\mathcal{B} := V^\perp$ is actually a MASA. However, it is not even clear whether it is an algebra (that is, whether it is closed for multiplication). There are two things though that are rather evident. First, that $\mathbb{1} \in \mathcal{B}$. Second, that \mathcal{B} is a self-adjoint subspace: $X \in \mathcal{B} \Leftrightarrow X^* \in \mathcal{B}$. This second property follows easily from the fact that it holds for $\mathcal{A}_1, \dots, \mathcal{A}_d$ and that the restriction of the Hilbert-Schmidt scalar product onto the real subspace of self-adjoints is real.

Lemma 3.1. *Let $K \subset M_d(\mathbb{C})$ be a self-adjoint linear subspace containing $\mathbb{1} \in M_d(\mathbb{C})$, and further let E_K stand for the ortho-projection onto K . Then K is a subalgebra of $M_d(\mathbb{C})$ if and only if E_K is 2-positive.*

Proof. First let us note that E_K automatically preserves the trace:

$$(3.1) \quad \text{Tr}(E_K(X)) = \langle \mathbb{1}, E_K(X) \rangle = \langle E_K(\mathbb{1}), X \rangle = \langle \mathbb{1}, X \rangle = \text{Tr}(X).$$

Now if K is a subalgebra of $M_d(\mathbb{C})$, then E_K is the trace-preserving conditional expectation onto K whose *complete* positivity is well-known. *Vice versa*, if E_K is 2-positive, then by [27, Corollary 2.8] one has the operator inequality

$$(3.2) \quad E_K(X^*X) \geq E_K(X^*)E_K(X).$$

In particular, if $X \in K$, then $E_K(X^*X) \geq X^*X$ and by applying the trace on both sides one further sees that it is actually an equality: $E_K(X^*X) = X^*X = E_K(X^*)E_K(X)$. Then by [27, Theorem 3.1] it follows that K is in the *multiplicative domain* of E_K . Hence if $X, Y \in K$, then $XY = E_K(X)E_K(Y) = E_K(XY) \in K$, showing that K is a subalgebra of $M_d(\mathbb{C})$. \square

Lemma 3.2. *Let B_1, \dots, B_n be an ONB in \mathcal{B} . Then $E_{\mathcal{B}}(X) = \sum_k B_k^* X B_k$ for all $X \in M_d(\mathbb{C})$, where $E_{\mathcal{B}}$ is the ortho-projection onto \mathcal{B} .*

Proof. Let us fix an ONB $A_1^{(k)}, \dots, A_{d-1}^{(k)}$ in $(\mathcal{A}_k \cap \{\mathbb{1}\}^\perp)$ for each $k = 1, \dots, d$. Then, on the one hand, $A_1^{(k)}, \dots, A_{d-1}^{(k)}, \frac{1}{\sqrt{d}}\mathbb{1}$ is an ONB in \mathcal{A}_k . On the other hand, the $d(d-1)$ elements, $A_j^{(k)}$ ($k = 1, \dots, d; j = 1, \dots, d-1$), together with B_1, \dots, B_d , form an ONB in the full space $M_d(\mathbb{C})$. So, on the one hand, by formula (2.7) we have that

$$(3.3) \quad \sum_j (A_j^{(k)})^* X A_j^{(k)} + \frac{1}{\sqrt{d}} \mathbb{1} X \frac{1}{\sqrt{d}} \mathbb{1} = E_{\mathcal{A}_k}(X),$$

implying that $\sum_j (A_j^{(k)})^* X A_j^{(k)} = E_{\mathcal{A}_k}(X) - \frac{1}{d} X$. On the other hand, by Lemma 2.1,

$$(3.4) \quad \sum_n B_n^* X B_n + \sum_{k,j} (A_j^{(k)})^* X A_j^{(k)} = \text{Tr}(X) \mathbb{1}.$$

Hence

$$(3.5) \quad \sum_n B_n^* X B_n = \text{Tr}(X) \mathbb{1} - \sum_{k,j} (A_j^{(k)})^* X A_j^{(k)} = X - \sum_{k=1}^d (E_{\mathcal{A}_k}(X) - \frac{1}{d} \text{Tr}(X) \mathbb{1}).$$

But $\frac{1}{d} \text{Tr}(X) \mathbb{1} = \langle \frac{1}{\sqrt{d}} \mathbb{1}, X \rangle \frac{1}{\sqrt{d}} \mathbb{1} = E_{\mathbb{C}\mathbb{1}}(X)$. Thus $E_{\mathcal{A}_k}(X) - \frac{1}{d} \text{Tr}(X) \mathbb{1} = E_{\mathcal{A}_k}(X) - E_{\mathbb{C}\mathbb{1}}(X) = E_{(\mathcal{A}_k \cap \{\mathbb{1}\}^\perp)}(X)$, since $\mathbb{C} \subset \mathcal{A}_k$. So finally we obtain that

$$(3.6) \quad \sum_n B_n^* X B_n = X - \sum_k E_{(\mathcal{A}_k \cap \{\mathbb{1}\}^\perp)}(X) = (id - E_V)(X) = E_{V^\perp}(X) = E_{\mathcal{B}}(X)$$

since V is spanned by the d pairwise orthogonal subspaces $(\mathcal{A}_k \cap \{\mathbb{1}\}^\perp)$ ($k = 1, \dots, d$). \square

Proposition 3.3. *The subspace \mathcal{B} is a MASA.*

Proof. By our previous lemma, $E_{\mathcal{B}}$ is completely positive, so by Lemma 3.1, \mathcal{B} is an algebra. On the other hand, if $X' \in \mathcal{B}'$, then

$$(3.7) \quad E_{\mathcal{B}}(X') = \sum_{k=1}^d B_k^* X' B_k = X' \sum_{k=1}^d B_k^* B_k = X' E_{\mathcal{B}}(\mathbb{1}) = X',$$

showing that $\mathcal{B}' \subset \mathcal{B}$ and hence that \mathcal{B}' is abelian. Thus $\mathcal{B} = (\mathcal{B}')'$ is unitarily equivalent to the subalgebra of all block-diagonal matrices of $M_d(\mathbb{C})$ for some fixed

sequence of block sizes. However, $\dim(\mathcal{B}) = d$, so the only possibility is that all of these blocks are 1-dimensional, implying that \mathcal{B} is a MASA. \square

Corollary 3.4. *Suppose that $\mathcal{E}_1, \dots, \mathcal{E}_d$ is a collection of MUB in \mathbb{C}^d . Then there exists an ONB \mathcal{E}_{d+1} so that $\mathcal{E}_1, \dots, \mathcal{E}_d, \mathcal{E}_{d+1}$ is a complete collection of MUB.*

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