

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 given a collection of d MUB in \mathbb{C}^d can be always 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 $N(d) \leq d - 1$.

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

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

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 of the question is coming 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 evidences [5, 6] suggests that $N(6) = 3$, which is much less than 7 (that 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 [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 be always completed and the first example for this occurs in $d = 4$ dimensions; see [9]. This is in perfect similarity with the following. A collection of mutually orthogonal Latin squares “missing” only one element to

be complete can be indeed completed[†]. In general, a collection of mutually orthogonal $n \times n$ Latin squares “missing” two elements cannot be always completed and the smallest value[‡] (and by [14] infact 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 point of views. It may be considered to regard Lie algebra theory [15]. The original problem, which is formulated in a complex space, may be also 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 better to say: matrix algebras).

There is a natural way to associate a maximal abelian $*$ -subalgebra (in short: a MASA) to an orthonormed 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 (called “quasi-orthogonality”). Infact, in the study of matrix algebras one considers systems of quasi-orthogonal subalgebras *in general* (that is, systems consisting of all kind of subalgebras — not only maximal abelian ones). For the topic of quasi-orthogonal subalgebras (or, as it is sometimes called: complementary subalgebras) and its relation to mutual unbiasedness see for example [18, 19, 21, 20] and [22]. Note that apart from the finite dimensional case, quasi-orthogonal subalgebras were also considered in the context of type II_1 von Neumann algebras; see [23].

Suppose $\mathcal{A}_1, \dots, \mathcal{A}_d, \mathcal{A}_{d+1}$ is a complete collection of quasi-orthogonal MASAs in $M_d(\mathbb{C})$. Then \mathcal{A}_{d+1} must be the orthogonal complement of $V := +_{k=1}^d (\mathcal{A}_k \cap \{\mathbb{1}\}^\perp)$. So if we are only given d quasi-orthogonal MASAs, then only at one place we can possibly find a MASA which is quasi-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 infact a MASA, which is exactly what will be done in this work.

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 need to diagonalize; in particular we need to find 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

$$\mathcal{A}_{\mathcal{E}} = \text{Span}\{P_{\mathbf{e}_j} \mid j = 1, \dots, d\}, \quad (2)$$

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 $\mathcal{A} = \mathcal{A}_{\mathcal{E}}$.

[†]This is well-known to experts of the field [10], but it is difficult to give a good reference. One may say that it is 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.

[‡]It 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 were already known to Euler and in [13] it is proved that for any $n \geq 4$ there exists a bachelor Latin square.

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

$$\langle A, B \rangle = \text{Tr}(A^*B) \quad (A, B \in M_d(\mathbb{C})). \quad (3)$$

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

$$E_{\mathcal{A}_{\mathcal{E}}}(X) = \sum_{k=1}^d P_{\mathbf{e}_k} X P_{\mathbf{e}_k} \quad (4)$$

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 **quasi-orthogonal**. A direct consequence of the definitions of the Hilbert-Schmidt scalar product and of quasi-orthogonality is that \mathcal{A} and \mathcal{B} are quasi-orthogonal subalgebras of $M_d(\mathbb{C})$ if and only if for all $A \in \mathcal{A}$ and $B \in \mathcal{B}$,

$$\tau(AB) = \tau(A)\tau(B), \quad (5)$$

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 (5) — two MASAs $\mathcal{A}_{\mathcal{E}}$ and $\mathcal{A}_{\mathcal{F}}$ in $M_d(\mathbb{C})$ are quasi-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 quasi-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

$$\frac{d^2 - 1}{d - 1} = d + 1 \quad (6)$$

pairwise orthogonal, $(d - 1)$ -dimensional subspaces. So when $d > 1$, a collection of quasi-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 ortho-normed bases in $M_d(\mathbb{C})$. Its proof can be found for example in [24]; but one could also have a look at [25, Proposition 1], which is a stronger generalization. However, for self-containment let us see now 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} 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

$$\sum_{k=1}^{d^2} B_k^* X B_k = \sum_{k,j,l=1}^{d^2} (\lambda_{k,j} A_j)^* X (\lambda_{k,l} A_k) = \sum_{k,j,l=1}^{d^2} \overline{\lambda_{k,j}} \lambda_{k,l} A_j^* X A_l = \sum_{j=1}^{d^2} A_j^* X A_j \quad (7)$$

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”.

Note that the same argument, together with formula (4), 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

$$E_{\mathcal{A}}(X) = \sum_k A_k^* X A_k. \quad (8)$$

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 quasi-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 $V := +_k^d (\mathcal{A}_k \cap \{\mathbb{1}\}^\perp)$ 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 the multiplication). There are two things though, that are rather evident. First, that $\mathbb{1} \in \mathcal{B}$. Second, that \mathcal{B} has an ONB consisting of self-adjoint elements only; an easy exercise shows that this follows 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 (so infact we could consider the whole construction just in the real subspace of self-adjoints).

Lemma 3.1. *Let B_1, \dots, B_n 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 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 one hand, by formula (8) we have that

$$\sum_j (A_j^{(k)})^* X A_j^{(k)} + \frac{1}{\sqrt{d}} \mathbb{1} X \frac{1}{\sqrt{d}} \mathbb{1} = E_{\mathcal{A}_k}(X), \quad (9)$$

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,

$$\sum_n B_n^* X B_n + \sum_{k,j} (A_j^{(k)})^* X A_j^{(k)} = \text{Tr}(X) \mathbb{1}. \quad (10)$$

Hence

$$\sum_n B_n^* X B_n = \text{Tr}(X) \mathbb{1} - \sum_{k,j} (A_j^{(k)})^* X A_j^{(k)} = X - \sum_{k=1}^d (E_{\mathcal{A}_k}(X) - \frac{1}{d} \text{Tr}(X) \mathbb{1}). \quad (11)$$

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 $\sum_n B_n^* X B_n =$

$$= X - \sum_k E_{(\mathcal{A}_k \cap \{\mathbb{1}\}^\perp)}(X) = (id - E_V)(X) = E_{V^\perp}(X) = E_{\mathcal{B}}(X) \quad (12)$$

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

Proposition 3.2. *Elements in \mathcal{B} commute.*

Proof. It is clear that to justify our claim it is enough to show that if B_1, \dots, B_d is an ONB in \mathcal{B} consisting of self-adjoints only, then a self-adjoint element $R \in \mathcal{B}$ must commute with every B_k for $k = 1, \dots, d$. We even may assume that R is a positive operator: $R \geq 0$, with its smallest eigenvalue being exactly zero. (Indeed, if $R \in \mathcal{B}$ is self-adjoint, then $\tilde{R} := R - t\mathbb{1}$ becomes such an operator if we set $t := \min(\text{Sp}(R))$ to be the smallest eigenvalue of R .) Then $\tilde{R} \in \mathcal{B}$ since $\mathbb{1} \in \mathcal{B}$ and of course something commutes with R if and only if it commutes with \tilde{R} .) By our previous lemma, taking account of the fact that $B_k^* = B_k$ and $R \in \mathcal{B}$, we have that

$$\sum_{k=1}^d B_k R B_k = R. \quad (13)$$

Of course $(\text{Ker}(X) \cap \text{Ker}(Y)) \subset \text{Ker}(X + Y)$ for any two operators X and Y , but in general, nothing more can be said. However, if X and Y are positive operators, then the previous inclusion is infact an equality. Looking at the above sum, we see that each term is evidently positive, implying, by what was said, that $\text{Ker}(R) \subset \text{Ker}(B_k R B_k)$ for each $k = 1, \dots, d$. So let $\mathbf{x} \in \text{Ker}(R)$ and set $\mathbf{y} := B_k \mathbf{x}$. Then $\mathbf{x} \in \text{Ker}(B_k R B_k)$ so

$$0 = \langle \mathbf{x}, B_k R B_k \mathbf{x} \rangle = \langle B_k \mathbf{x}, R B_k \mathbf{x} \rangle = \langle \mathbf{y}, R \mathbf{y} \rangle \quad (14)$$

implying that $\mathbf{y} \in \text{Ker}(R)$, too. (Recall that for a positive operator $R \geq 0$ one has the equality $\text{Ker}(R) = \{\mathbf{y} \mid \langle \mathbf{y}, R \mathbf{y} \rangle = 0\}$.) So $B_k(\text{Ker}(R)) \subset \text{Ker}(R)$ for every $k = 1, \dots, d$.

Let us denote the spectral projection of R corresponding to the eigenvalue 0 (so actually: the ortho-projection onto $\text{Ker}(R)$) by P_0 . Then, by what we have obtained, $B_k P_0 = P_0 B_k P_0$ so

$$P_0 B_k = (B_k P_0)^* = (P_0 B_k P_0)^* = P_0 B_k P_0 = B_k P_0 \quad (15)$$

that is, P_0 commutes with B_k for every $k = 1, \dots, d$.

If R was the zero operator, then of course we are finished. If not, then it has at least one more eigenvalue apart from zero. Let then $\tilde{R} := R - \lambda\mathbb{1} + (\mu + 1)P_0$, where $\lambda := \min(\text{Sp}(R) \setminus \{0\})$ is the second smallest eigenvalue of R and $\mu := \max(\text{Sp}(R)) \geq \lambda$ is the largest eigenvalue. Note that \tilde{R} is still a positive operator with its smallest eigenvalue being zero and that its eigenspace associated to 0 is exactly the eigenspace of R associated to its second smallest eigenvalue λ .

Since $\mathbb{1} \in \mathcal{B}$, we have that $\sum_k B_k^2 = \sum_k B_k \mathbb{1} B_k = \mathbb{1}$. Hence by the obtained commutation relation regarding P_0 , we have that

$$E_{\mathcal{B}}(\tilde{R}) = \sum_{k=1}^d B_k \tilde{R} B_k = R + (\lambda\mathbb{1} - \mu P_0) \sum_{k=1}^d B_k^2 = \tilde{R}. \quad (16)$$

This shows that $\tilde{R} \in \mathcal{B}$ and hence that $P_0 \in \mathcal{B}$, too. Repeating our argument with R replaced by \tilde{R} , we get that the spectral projection P_λ associated to the second smallest eigenvalue λ is also in \mathcal{B} and that P_λ commutes with B_k for all $k = 1, \dots, d$. Proceeding in a similar manner, by induction we get that B_k ($k = 1, \dots, d$) commutes with every spectral projection of R , and hence, that with R , too.

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

Proof. Let us choose again an ONB B_1, \dots, B_n in \mathcal{B} consisting of self-adjoint elements, only. Since they pairwise commute, they can be jointly diagonalized by a unitary operator: there exists a unitary U such that $U^* B_k U$ is a diagonal matrix for all $k = 1, \dots, d$. This means that

$$\text{Span}\{U^* B_k U \mid k = 1, \dots, d\} = U^* \text{Span}(B_k \mid k = 1, \dots, d) U = U^* \mathcal{B} U \quad (17)$$

is a subspace of the diagonal matrices. However, since its dimension is d , it must coincide with the full space of diagonal matrices. So $U^* \mathcal{B} U$ is a MASA and hence \mathcal{B} is a MASA, too.

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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