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PRINCIPAL ANGLES AND APPROXIMATION FOR QUATERNIONIC PROJECTIONS

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This paper is dedicated to Professor Tsuyoshi Ando, in celebration of his expertise in matrix and operator theory

Communicated by G. Androulakis

ABSTRACT. We extend Jordan's notion of principal angles to work for two subspaces of quaternionic space, and so have a method to analyze two orthogonal projections in the matrices over the real, complex or quaternionic field (or skew field). From this we derive an algorithm to turn almost commuting projections into commuting projections that minimizes the sum of the displacements of the two projections. We quickly prove what we need using the universal real C^* -algebra generated by two projections.

1. TWO PROJECTIONS, THE THREE-FOLD WAY

The general form of two projections on complex Hilbert space is well-known, going back to at least Dixmier [6]. The real case is older, being implicit in the work of Jordan [13, §IV], where principal vectors and principal angles were introduced. From principal vectors one can derive the structure theorem for matrix projections, as is explained in the real case in [8]. Restricted to the finite-dimensional case, we can think of these as theorems about two projections in certain finite-dimensional real C^* -algebras. One would therefore expect the same result to hold in all finite-dimensional real C^* -algebras, and so in $\mathbf{M}_n(\mathbb{H})$ where \mathbb{H} is the skew field of quaternions.

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The following is very easy, given the machinery in developed by Sørensen in [19]. We call it a theorem only because so much follows from it that is not so obvious.

Theorem 2.1. *The universal R^* -algebra generated by two elements p and q subject to the relations $p^2 = p^* = p$ and $q^2 = q^* = q$ is*

$$\mathcal{B} = \left\{ f \in C\left([0, \frac{\pi}{2}], \mathbf{M}_2(\mathbb{R})\right) \mid f(0) \in \begin{bmatrix} \mathbb{R} & 0 \\ 0 & 0 \end{bmatrix} \text{ and } f(1) \in \begin{bmatrix} \mathbb{R} & 0 \\ 0 & \mathbb{R} \end{bmatrix} \right\}$$

and the universal generators are p_0 and q_0 where

$$p_0(t) = P_t, \quad q_0(t) = Q_t. \tag{2.1}$$

Proof. The complexification of \mathcal{B} is clearly

$$\mathcal{A} = \left\{ f \in C\left([0, \frac{\pi}{2}], \mathbf{M}_2(\mathbb{C})\right) \mid f(0) \in \begin{bmatrix} \mathbb{C} & 0 \\ 0 & 0 \end{bmatrix} \text{ and } f(1) \in \begin{bmatrix} \mathbb{C} & 0 \\ 0 & \mathbb{C} \end{bmatrix} \right\}$$

and this is known to be the universal complex C^* -algebra for the relations of being two orthogonal projections. For example, see [17, §3]. By [19, Theorem 5.2.6.], the universal R^* -algebra for these relations is the closed real $*$ -algebra in \mathcal{A} generated by $\{p_0, q_0\}$, which is \mathcal{B} . \square

2.1. Proof of Theorem 1.1. Every finite-dimensional quotient of \mathcal{B} is of the form

$$\mathcal{C} = \mathbf{M}_2(\mathbb{R}) \oplus \cdots \oplus \mathbf{M}_2(\mathbb{R}) \oplus \mathbb{R} \oplus \cdots \oplus \mathbb{R}$$

with any number of the $\mathbf{M}_2(\mathbb{R})$ and up to two of the \mathbb{R} , with the surjection from \mathcal{B} being evaluation at various t in $[0, 1)$ and also

$$f \mapsto \begin{bmatrix} 1 & 0 \end{bmatrix} f(1) \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

or

$$f \mapsto \begin{bmatrix} 0 & 1 \end{bmatrix} f(1) \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

The $*$ -homomorphisms between finite-dimensional R^* -algebras are known, say by [9]. Up to unitary equivalence, the only embedding of \mathcal{C} into $\mathbf{M}_n(\mathbb{H})$ is found be the obvious embedding into

$$\mathcal{D} = \mathbf{M}_2(\mathbb{H}) \oplus \cdots \oplus \mathbf{M}_2(\mathbb{H}) \oplus \mathbb{H} \oplus \cdots \oplus \mathbb{H}$$

followed by an embedding that puts the $\mathbf{M}_k(\mathbb{H})$ down the diagonal, perhaps with multiplicity in each summand.

2.2. Computing principal vectors. The standard for computing principal angles and vectors is an algorithm by Björck and Golub [4]. Let us assume our subspaces are given as the ranges of projections P and Q . Their algorithm first obtains partial isometries E and F so that $EE^* = P$ and $FF^* = Q$. Then a singular value decomposition $U\Omega V^*$ of E^*F is computed, and the principal vectors are found by pairing each column from EU with a column from FV .

We describe here a different algorithm. We have no particular application in mind, so do not explore speed or accuracy issues. Moreover, the algorithm is simpler if it is restricted to the case $\|P - Q\| \leq 1/\sqrt{2}$. We use always the

operator norm, so $\|X\|$ is the largest singular value of X . See [15] for details regarding the norm in the case of a matrix of quaternions.

Following an idea from [18], we let U be the unitary in the polar decomposition of $X = QP + (I - Q)(I - P)$. We take an orthonormal basis of eigenvectors for PQP , and for each \mathbf{v} in that basis coming from an eigenspace at or above $\frac{1}{2}$ we find that $(\mathbf{v}, U\mathbf{v})$ is a pair of principal vectors. Assuming the eigen-decomposition is done with the appropriate symmetry respected, the result will have the correct symmetry.

This algorithm can be validated, in exact arithmetic, from Theorem 1.1. Notice that the condition $\|P - Q\| \leq 1/\sqrt{2}$ causes the θ_j to be at most $\frac{\pi}{4}$. For each $P = P_\theta$ and $Q = Q_\theta$ we note that

$$X = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix} \begin{bmatrix} \cos(\theta) & 0 \\ 0 & \cos(\theta) \end{bmatrix}$$

so

$$U = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix}$$

and the eigenvector for

$$PQP = \begin{bmatrix} \cos^2(\theta) & 0 \\ 0 & 0 \end{bmatrix}$$

for an eigenvalue above one-half will be

$$\begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

and this will get paired with

$$\begin{bmatrix} \cos(\theta) \\ \sin(\theta) \end{bmatrix}.$$

Notice that X will be invertible, and indeed have $\|X\| \leq 1$ and $\|X^{-1}\| \leq \sqrt{2}$. Thus U can be quickly and accurately computed by Newton's method [12].

Since we are limiting our inputs to the case $\|p - q\| \leq 1/\sqrt{2}$ we know that five iterations in Newton's method will suffice, where $X_0 = X$ and each iteration sets X_{1+i} equal to $\frac{1}{2}(X_n + (X_n^*)^{-1})$. An analysis of the singular values of X_n shows they are between C_n and 1 where $C_0 = 1/\sqrt{2}$ and $C_{n+1} = \frac{1}{2}(C_n + C_n^{-1})$. Since C_5 will be within machine precision of 1 we conclude that X_5 is as close to being unitary as we can expect.

A faster and more useful algorithm will be found by using the best algorithms for finding the unitary part in the polar decomposition of X , be it real, complex or quaterionic, dense or sparse, well-conditioned or not. If we allow $\|P - Q\| = 1$ then the theory tells us we need to find eigenvectors for all positive eigenvalues of X . Since X will not be invertible the techniques for polar decomposition will not be as easy.

We now present the algorithm as pseudocode, assuming that p and q are the projection matrices with $\|p - q\| \leq 1/\sqrt{2}$.

$$\begin{aligned} d &\leftarrow \text{Tr}(p) \\ u &\leftarrow qp - (I - p)(I - q) \end{aligned}$$

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for j = 1 to 5
    u ← (½(u + (u*)-1))
end
{a1...ad} ← eigenvectors for top d eigenvalues of pqp
for j = 1 to d
    bj ← Uaj
end

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The pairs of principal vectors are in the \mathbf{a}_j and \mathbf{b}_j . The eigensolver used should give an orthogonal set of eigenvectors, and in the real case should give real eigenvectors.

Code that tests this algorithm is available at the “Lobo Vault” at the University of New Mexico [16]. For this algorithm to work in the quaternionic case, it needs an eigensolver that finds a symplectic unitary diagonalization (or partial diagonalization) of a matrix that is both hermitian and quaternionic. See [11, §9.1] and [3] for information on how to build such an eigensolver.

3. ALMOST COMMUTING PROJECTIONS

Almost commuting projections are much easier to understand than almost commuting hermitian contractions. Indeed, Lin’s theorem [14] is sufficiently difficult that there are no algorithms implementing it. An algorithm for a related problem might be helpful.

We can easily impose on our universal real C^* -algebra a relation that bounds the commutator.

Corollary 3.1. *Suppose $0 \leq \delta < \frac{1}{2}$. Let $C = \frac{1}{2} \arcsin(2\delta)$. The universal R^* -algebra generated by two elements p and q subject to the relations $p^2 = p^* = p$ and $q^2 = q^* = q$ and*

$$\|pq - qp\| \leq \delta$$

is

$$\mathcal{B}_\delta = \left\{ f \in C(I_C, \mathbf{M}_2(\mathbb{R})) \mid f(0) \in \begin{bmatrix} \mathbb{R} & 0 \\ 0 & 0 \end{bmatrix} \text{ and } f(1) \in \begin{bmatrix} \mathbb{R} & 0 \\ 0 & \mathbb{R} \end{bmatrix} \right\}$$

where $I_C = [0, C] \cup [\frac{\pi}{2} - C, \frac{\pi}{2}]$ and the universal generators are p_0 and q_0 as in equation (2.1).

If P and Q almost commute, and we have candidates P' and Q' that are commuting projections, we can hope to have minimized either

$$\|P' - P\| + \|Q' - Q\|$$

or

$$\max(\|P' - P\|, \|Q' - Q\|)$$

for any given value of $\delta = \|[P, Q]\|$. In the first case, we can just let $P' = P$ and set Q' to be the spectral projection for $[\frac{1}{2}, \infty)$ of

$$PQP + (I - P)Q(I - P).$$

This leads to the well-known result for the sum of displacements, namely

$$\|P' - P\| + \|Q' - Q\| = \sin\left(\frac{1}{2} \arcsin(2\delta)\right).$$

Controlling the max of the displacements does not seem to have been considered before. We observe that for $0 \leq \theta \leq \pi/4$,

$$\left\|P_\theta - Q_{\frac{\theta}{2}}\right\| = \left\|Q_\theta - Q_{\frac{\theta}{2}}\right\| = \sin\left(\frac{\theta}{2}\right)$$

while for $\pi/4 \leq \theta \leq \pi/2$, we let $\theta' = \frac{\theta}{2} + \frac{\pi}{4}$ and observe

$$\|P_\theta - (I - Q_{\theta'})\| = \|Q_\theta - Q_{\theta'}\| = \sin\left(\frac{\theta}{2}\right).$$

For all θ we find

$$\|P_\theta Q_\theta - Q_\theta P_\theta\| = \frac{1}{2} \sin(2\theta).$$

Finally, when we start with 0 and 1, or 0 and 0, we just leave those alone.

Theorem 3.2. *Suppose \mathbb{A} equals \mathbb{R} , \mathbb{C} or \mathbb{H} . If P and Q are projections in $\mathbf{M}_n(\mathbb{A})$ then there are projections P' and Q' in $\mathbf{M}_n(\mathbb{A})$ that commute and so that*

$$\|P - P'\| = \|Q - Q'\| = \sin\left(\frac{1}{4} \arcsin(2\delta)\right)$$

where

$$\delta = \|PQ - QP\|.$$

The choice of P' and Q' can be made so that it is continuous in P and Q .

Proof. We can simply work in \mathcal{B}_δ and use the well-known fact that naturality in C^* -algebra constructions leads to continuity. \square

Theorem 3.3. *For $\delta = \|PQ - QP\| < \frac{1}{2}$, the commuting projections P' and Q' of Theorem 3.2 can be computed by the following formulas: let*

$$\begin{aligned} R &= \frac{1}{2} (PQP + QPQ) \\ S &= \frac{1}{2} ((I - P)Q(I - P) + Q(I - P)Q) \\ T &= PQP + (I - P)(I - Q)(I - P) \end{aligned}$$

and then let E_R and E_S be the spectral projections for R and S corresponding to the set $[\frac{1}{3}, \infty)$ and E_T the spectral projections for T corresponding to the set $[\frac{1}{2}, \infty)$, and finally

$$P' = E_T E_R E_T + (I - E_T)(I - E_S)(I - E_T) \quad (3.1)$$

$$Q' = E_T E_R E_T + (I - E_T)E_S(I - E_T) \quad (3.2)$$

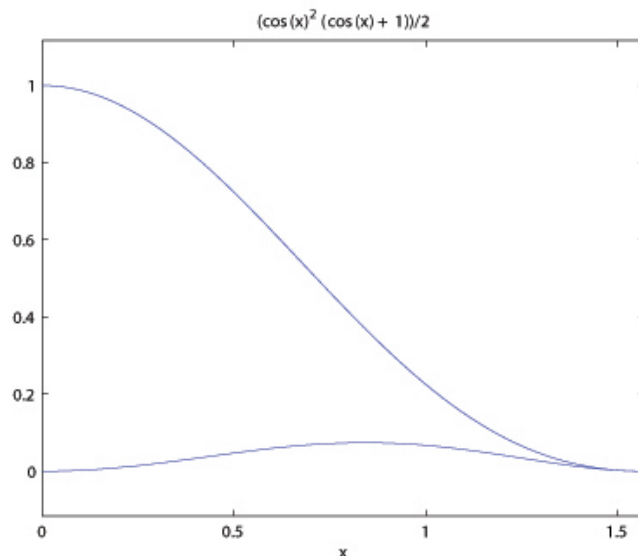


FIGURE 1. The two eigenvalues of $r(x)$ for various scalar values of x .

Proof. We notice that when $0 \leq x \leq \frac{\pi}{4}$, if we set

$$R = \frac{1}{2} (P_x Q_x P_x + Q_x P_x Q_x)$$

then

$$R = \begin{bmatrix} \cos\left(\frac{x}{2}\right) & \sin\left(\frac{x}{2}\right) \\ \sin\left(\frac{x}{2}\right) & -\cos\left(\frac{x}{2}\right) \end{bmatrix} \begin{bmatrix} \lambda_1(x) & 0 \\ 0 & \lambda_2(x) \end{bmatrix} \begin{bmatrix} \cos\left(\frac{x}{2}\right) & \sin\left(\frac{x}{2}\right) \\ \sin\left(\frac{x}{2}\right) & -\cos\left(\frac{x}{2}\right) \end{bmatrix}$$

where

$$\lambda_1(x) = \cos^2(x) \left(\frac{1}{2} + \frac{1}{2} \cos(x) \right)$$

and

$$\lambda_2(x) = \cos^2(x) \left(\frac{1}{2} - \frac{1}{2} \cos(x) \right).$$

Suppose e_r is the spectral projection of r for $[\frac{1}{3}, \infty)$. Since

$$\lambda_2(x) \leq \lambda_2\left(\frac{\pi}{4}\right) = \frac{2 - \sqrt{2}}{8} \leq \frac{1}{3} \leq \frac{2 + \sqrt{2}}{8} = \lambda_1\left(\frac{\pi}{4}\right) \leq \lambda_1(x)$$

we find that

$$E_R = \begin{bmatrix} \cos^2\left(\frac{x}{2}\right) & \sin\left(\frac{x}{2}\right) \cos\left(\frac{x}{2}\right) \\ \sin\left(\frac{x}{2}\right) \cos\left(\frac{x}{2}\right) & \sin^2\left(\frac{x}{2}\right) \end{bmatrix}$$

which is on the midpoint of the canonical path between P_x and Q_x . (See [5].) By symmetry, set

$$S = \frac{1}{2} ((1 - P_x)Q_x(1 - P_x) + Q_x(1 - P_x)Q_x)$$

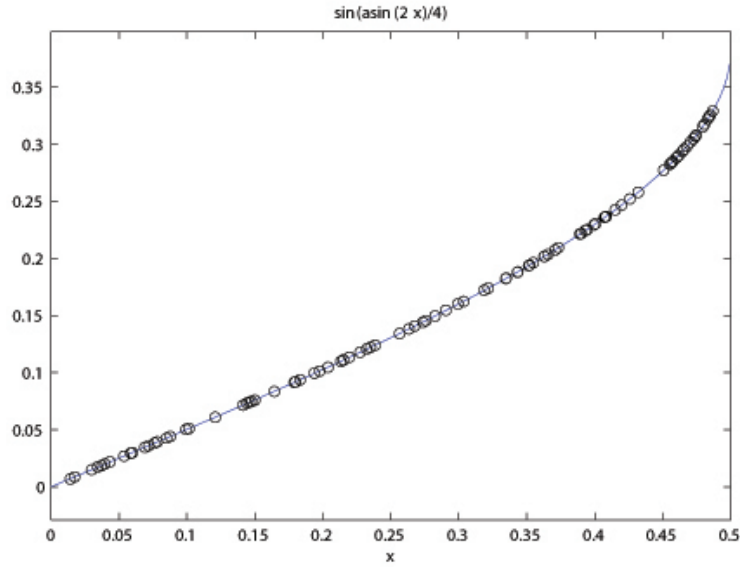


FIGURE 2. Distance to computed commuting projections by the Formulas Theorem 3.3, implemented in Matlab. There were 100 test pairs of 200-by-200 real projections of distance at most 0.49 apart. The solid curve is the exact answer of $\sin(\arcsin(2\delta)/4)$.

and find that the spectral projection E_S of S for $[\frac{1}{5}, \infty)$ satisfies

$$E_S = \begin{bmatrix} \sin^2\left(\frac{x}{2}\right) & \sin\left(\frac{x}{2}\right)\cos\left(\frac{x}{2}\right) \\ \sin\left(\frac{x}{2}\right)\cos\left(\frac{x}{2}\right) & \cos^2\left(\frac{x}{2}\right) \end{bmatrix}.$$

For $\frac{\pi}{4} \leq x \leq \frac{\pi}{2}$ this is the “midpoint” between $1 - P_x$ and Q_x .

These projections just constructed do not become zero when x is in the opposite subinterval, as indicated by Figure 1. This is the reason we need T and its spectral projections.

For all x we use

$$T = P_x Q_x P_x + (1 - P_x)(1 - Q_x)(1 - P_x)$$

which is

$$T = \begin{bmatrix} \cos^2(x) & 0 \\ 0 & \sin^2(x) \end{bmatrix}.$$

Thus the spectral projection E_T for T corresponding to $[\frac{1}{2}, \infty)$ is

$$\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$

for x less than $\frac{\pi}{2}$, and is

$$\begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

for x greater than $\frac{\pi}{2}$.

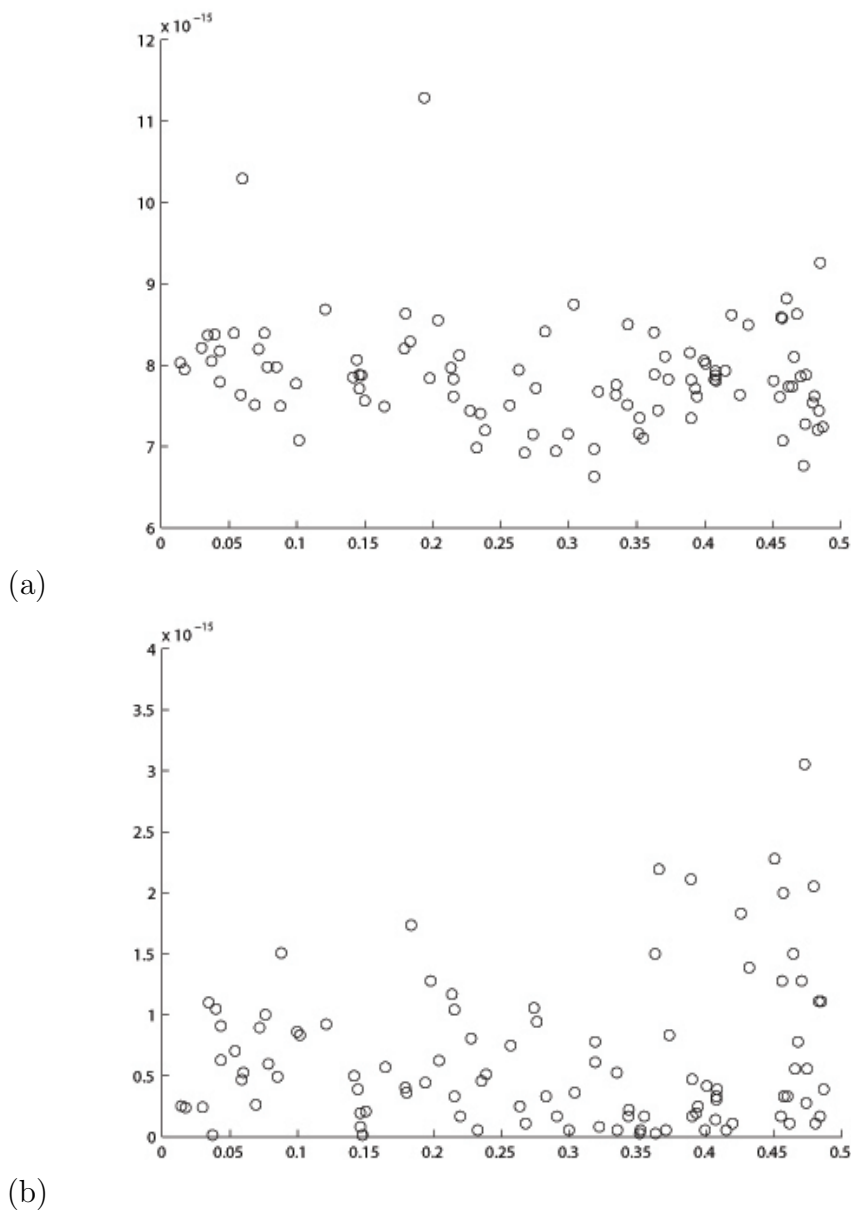


FIGURE 3. The errors with the same test matrices as in Figure 2. (a) The sum of errors, in operator norm, in the relations $P'^2 = P', Q'^2 = Q', P'^* = P', Q'^* = Q'$ and $P'Q' = Q'P'$. (b) The errors from the optimal in $\max(\|P' - P\|, \|Q' - Q\|)$.

For any x , if we define now P' and Q' by (3.1) and (3.1) then these are exactly commuting projections and

$$\max(\|P_x - P'\|, \|Q_x - Q'\|) = \sin\left(\frac{x}{2}\right).$$

Since

$$\delta = \|P_x Q_x - P_x Q_x\| = \sin(x) \cos(x) = \frac{1}{2} \sin(2x)$$

we have

$$\max(\|P_x - P'\|, \|Q_x - Q'\|) = \sin\left(\frac{1}{4} \arcsin(2\delta)\right).$$

This completes the proof in the 2-by-2 case. The general case follows, by Theorem 1.1. \square

Some applications of the half-angle formula give us

$$\sin\left(\frac{1}{4} \arcsin(2\delta)\right) = \sqrt{\frac{1}{2} - \frac{1}{2} \sqrt{\frac{1}{2} + \frac{1}{2} \sqrt{1 - 4\delta^2}}}$$

should someone think this is an improvement.

The formulas in Theorem 3.3 are readily programmable for complex matrices, and can be done so that real or quaternionic matrices lead to real or quaternionic matrices during the calculation. Code that tests this for real matrices is available [16]. The results are shown in Figure 2 with numerical errors shown in Figure 3. The data as shown were created with `testCommute(200,100)` using the code in the auxiliary file `testCommute.m`.

4. DISCUSSION

The motivation for this work was to have a complete solution to the almost commuting projections problem, including an algorithm, that might be useful when exploring the much deeper question of almost commuting hermitian matrices, be they real, complex or quaternionic. What makes this a relatively easy problem is that we can identify a universal real C^* -algebra associated to two projections. This universal algebra makes it easy to define principal angles between quaternionic subspaces.

A result that is closely related to the study of two projections concerns a single idempotent in a C^* -algebra.

Theorem 4.1. *The universal C^* -algebra for a single generator a and the relations*

$$\begin{aligned} a^2 &= a \\ \|a\| &\leq C \end{aligned}$$

is

$$\mathcal{I}_D = \left\{ f \in C([0, D], \mathbf{M}_2(\mathbb{C})) \mid f(0) \in \begin{bmatrix} \mathbb{C} & 0 \\ 0 & 0 \end{bmatrix} \right\}$$

via the isomorphism specified by

$$a \mapsto \begin{bmatrix} 1 & 0 \\ t & 0 \end{bmatrix},$$

where $D = \sqrt{C - 1}$.

This is implicit in the work of Afriat [2]. One assumes that Theorem 4.1 can be trivially modified to give the universal real C^* -algebra for an idempotent with norm at most C . It is likely then that Ando's results in [1] will work on real Hilbert space, relating an unbounded idempotent to its range and kernel orthoprojections.

There are other directions one can go with either Theorem 2.1 or the presumed real version of Theorem 4.1. Many standard results about projections and idempotents should now follow for real C^* -algebras.

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