

On vector configurations that can be realized in the cone of positive matrices

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Abstract

Let $\mathbf{v}_1, \dots, \mathbf{v}_n$ be n vectors in an inner product space. Can we find a $d \in \mathbb{N}$ and positive (semidefinite) matrices $A_1, \dots, A_n \in M_d(\mathbb{C})$ such that $\text{Tr}(A_k A_l) = \langle \mathbf{v}_k, \mathbf{v}_l \rangle$ for all $k, l = 1, \dots, n$? For such matrices to exist, one must have $\langle \mathbf{v}_k, \mathbf{v}_l \rangle \geq 0$ for all $k, l = 1, \dots, n$. We prove that if $n < 5$ then this trivial necessary condition is also a sufficient one and find an appropriate example showing that from $n = 5$ this is not so — even if we allowed realizations by positive operators in a von Neumann algebra with a faithful normal tracial state.

The fact that the first such example occurs at $n = 5$ is similar to what one has in the well-investigated problem of *positive factorization* of positive (semidefinite) matrices. If the matrix $(\langle \mathbf{v}_k, \mathbf{v}_l \rangle)_{(k,l)}$ has a positive factorization, then matrices A_1, \dots, A_n as above exist. However, as we show by a large class of examples constructed with the help of the Clifford algebra, the converse implication is false.

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1 Introduction

1.1 Motivation

Throughout this paper, the term “positive matrix” will mean “positive semidefinite matrix”. The aim of the paper is to study a geometrical property of the cone \mathcal{C}_d of positive matrices in $M_d(\mathbb{C})$ in the “large dimensional limit”: we investigate if a given configuration of vectors can be embedded in \mathcal{C}_d for *some* (possibly very large) $d \in \mathbb{N}$. Note that for $d_1 \leq d_2$ we have $\mathcal{C}_{d_1} \hookrightarrow \mathcal{C}_{d_2}$ in a natural manner, so if a configuration can be embedded in \mathcal{C}_{d_1} , then it can be embedded in \mathcal{C}_{d_2} .

To explain the precise meaning of our question, consider the real vector space formed by the self-adjoint elements of $M_d(\mathbb{C})$. It has a natural inner product defined by the formula

$$\langle A, B \rangle \equiv \frac{1}{d} \text{Tr}(AB) \quad (A^* = A, B^* = B \in M_d(\mathbb{C})), \quad (1)$$

making it a *Euclidean* space. Our cone \mathcal{C}_d is a convex cone in this space with a “sharp end-point” at zero¹: if $A, B \in \mathcal{C}_d$ then $\langle A, B \rangle \geq 0$.

Suppose we are given n vectors $\mathbf{v}_1, \dots, \mathbf{v}_n$ in a Euclidean space. Embedding them in an inner product preserving way in \mathcal{C}_d means finding n positive matrices $A_1, \dots, A_n \in \mathcal{C}_d$ such that

$$\langle \mathbf{v}_j, \mathbf{v}_k \rangle = \langle A_j, A_k \rangle \equiv \frac{1}{d} \text{Tr}(A_j A_k). \quad (2)$$

Since, as was mentioned, the angle between any two vectors in \mathcal{C}_d is $\leq \pi/2$, one can only hope to embed these vectors if $\langle \mathbf{v}_j, \mathbf{v}_k \rangle \geq 0$ for all $j, k = 1, \dots, n$. So suppose this condition is satisfied. Does it follow that the given vectors can be embedded in \mathcal{C}_d for some (possibly very large) d ? If not, can we characterize the configurations that can be embedded? To our knowledge, these questions have not been considered in the literature.

We postpone the summary of our results to the next subsection and note that there is a well-investigated problem — namely the problem of *positive factorization* — which has some relation to our questions. The relation between the two topics will also be discussed in the next subsection; here we shall only explain our original motivation.

If A is positive and $A \neq 0$, then $\text{Tr}(A) > 0$, so the affine hyperplane $\{X : \text{Tr}(X) = 1\}$ intersects each ray of the cone \mathcal{C}_d exactly once and geometric properties of this cone can be equally well studied by considering just the intersection

$$\mathcal{S}_d = \{A \in M_d(\mathbb{C}) : A \geq 0, \text{Tr}(A) = 1\}. \quad (3)$$

The compact convex body \mathcal{S}_d is usually referred to as the set of *density operators*, and it can be naturally identified with the set of states of $M_d(\mathbb{C})$. Many problems in quantum information theory boil down to geometrical questions about \mathcal{S}_d . From our point of view a relevant example is the famous open problem about *mutually unbiased bases*, which turned

¹Actually one has the much stronger property that an element X in this space belongs to the cone \mathcal{C}_d if and only if $\langle X, A \rangle \geq 0$ for all $A \in \mathcal{C}_d$; i.e. \mathcal{C}_d is a *self-dual* cone.

out [1] to be equivalent to asking whether a certain polytope — similarly to our question — can be embedded in \mathcal{S}_d or not. Though some properties of \mathcal{S}_d have been determined (e.g. its volume and surface [2] is known), its exact “shape” is still little understood.

However, rather than studying the geometry of \mathcal{C}_d (or \mathcal{S}_d) for a certain d , here we are more interested in the “large dimensional” behaviour. Indeed, often this is what matters; think for example of the topic of *operator monotonuous functions*. (The ordering between self-adjoint elements is determined — in some sense — by the geometry of \mathcal{C}_d , since the operator inequality $A \geq B$ simply means that $A - B \in \mathcal{C}_d$.) Indeed, saying that a certain function $f : \mathbb{R} \rightarrow \mathbb{R}$ is monotonuous (increasing) but *not* operator monotonuous means that though $f(x) \leq f(y)$ for all real $x \leq y$, there exist two (possibly very large) self-adjoint matrices $X \leq Y$ such that $f(X) \not\leq f(Y)$.

A more direct motivation for our question is the *Connes embedding conjecture*. This conjecture — in its original form — is about *finite* von Neumann algebras; i.e. von Neumann algebras having a normal faithful tracial state. According to Connes, it should be always possible to embed such a von Neumann algebra into an ultrapower \mathcal{R}^ω of the hyperfinite II_1 -factor \mathcal{R} in a trace-preserving way.

At first sight this might seem unrelated to our problem. However, this conjecture has many different (but equivalent) forms. For example, it is well-known that this embedding property holds if and only if moments of a finite set of self-adjoint elements from such a von Neumann algebra \mathcal{M} can always be “approximated” by those of a set of (complex, self-adjoint) matrices. (See e.g. [3, Prop. 3.3] for a proof.) Here by “approximation” we mean that for every $n, m \in \mathbb{N}$, $\epsilon > 0$ and self-adjoint operators $A_1, \dots, A_n \in \mathcal{M}$ it is possible to find a $d \in \mathbb{N}$ and self-adjoint matrices $X_1, \dots, X_n \in M_d(\mathbb{C})$ such that

$$|\tau(A_{j_1} \dots A_{j_s}) - \tau_d(X_{j_1} \dots X_{j_s})| \leq \epsilon \quad (4)$$

holds for every $s \leq m$ and $j_1, \dots, j_s \in \{1, \dots, n\}$. Here τ is a (fixed) faithful, normal, tracial state on \mathcal{M} and $\tau_d = \frac{1}{d} \text{Tr}$ is the normalized trace on $M_d(\mathbb{C})$. Note that the Connes embedding conjecture can also be reformulated in terms of linear inequalities between moments [4]. This approach has recently resulted [5, 6] in new forms of the conjecture which are in some sense similar to Hilbert’s 17th problem and are formulated *entirely* in terms of moments of matrices (i.e. in a way which apparently does not involve von Neumann algebras other than those of finite matrices).

It is then natural to ask: what can we say about moments of self-adjoint matrices, in general? Of course, there is not too much to say about the first and second moments. The set of numbers $\{\text{Tr}(X_j) : j = 1, \dots, n\}$ can be any subset of \mathbb{R} and the only condition on the second moments is that the matrix $(\text{Tr}(X_j X_k))_{(j,k)}$ must have only real entries and must be positive, as it is the *Gram matrix* of X_1, \dots, X_n when these are viewed as vectors in a Euclidean space.

While the first two moments are too banal to be interesting, higher moments are too complicated to be fully understood. In this respect it seems a good way “in between” to study moments of the form $\text{Tr}(X_j^2 X_k^2)$. Though they are 4-moments, they can be also considered as 2-moments of the *positive* matrices $Y_j := X_j^2$ ($j = 1, \dots, n$), which again leads to our question.

1.2 Relation to positive factorization and main results

There is a certain type of configuration which can be embedded in the cone of positives in a trivial manner. Indeed, let $\mathbf{v}_1, \dots, \mathbf{v}_n$ be vectors from the *positive orthant* of \mathbb{R}^d ; i.e. vectors of \mathbb{R}^d with only nonnegative entries (in which case of course $\langle \mathbf{v}_k, \mathbf{v}_l \rangle \geq 0$ follows automatically for all $k, l = 1, \dots, n$). Then for each $k = 1, \dots, n$ let A_k be \sqrt{d} times the $d \times d$ diagonal matrix whose diagonal entries are simply the entries of $\mathbf{v}_k \in \mathbb{R}^d$ (listed in the same order). It is now trivial that the matrices A_k are positive and that $\langle A_k, A_l \rangle \equiv \frac{1}{d} \text{Tr}(A_k A_l) = \langle \mathbf{v}_k, \mathbf{v}_l \rangle$ for all $k, l = 1, \dots, n$.

Note that in the above realization all matrices commute. Actually a certain converse of this remark is also true: if a vector configuration can be realized by commuting elements of \mathcal{C}_d , then this configuration can be embedded in the positive orthant $\mathbb{R}_{\geq 0}^d$. This simply follows from the fact that a set of positive, commuting matrices can be simultaneously diagonalized and that all diagonal entries of positive matrices must be nonnegative.

No more than 4 vectors span at most a 4-dimensional space and in [9] it is proved that if $\mathbf{v}_1, \dots, \mathbf{v}_4 \in \mathbb{R}^4$ are such that $\langle \mathbf{v}_k, \mathbf{v}_l \rangle \geq 0$ for all $k, l = 1, \dots, 4$ then there exists an orthogonal transformation $O : \mathbb{R}^4 \rightarrow \mathbb{R}^4$ such that $O\mathbf{v}_1, \dots, O\mathbf{v}_4$ all lie in the positive orthant of \mathbb{R}^4 . It follows at once that any configuration of $n \leq 4$ vectors such that the angle between any two is $\leq \pi/2$ can be embedded in the cone \mathcal{C}_4 .

Another elementary observation is that *any* number of vectors $\mathbf{v}_1, \dots, \mathbf{v}_n$ spanning a no more than 2-dimensional space and satisfying $\langle \mathbf{v}_k, \mathbf{v}_l \rangle \geq 0$ for all $k, l = 1, \dots, n$ can be embedded in the positive orthant of \mathbb{R}^2 and hence also in the cone \mathcal{C}_2 . Thus a configuration, with all inner products nonnegative, which does not have a realization in \mathcal{C}_d for any $d \in \mathbb{N}$ must consist of at least 5 vectors and must span a space of dimension ≥ 3 . In fact, as we shall show in the last section, there exists a configuration of 5 vectors in \mathbb{R}^3 with all pairwise inner products nonnegative but with no realization in any cone \mathcal{C}_d ($d \in \mathbb{N}$). In connection to the Connes embedding conjecture it is interesting to note that — as we shall explain — this particular configuration cannot be embedded in the cone of positives of any finite von Neumann algebra.

An $n \times n$ matrix A is said to have a positive factorization iff there exists another (possibly non-square) matrix B such that all entries of B are nonnegative reals and $A = B^T B$. A trivial necessary condition for the existence of a positive factorization is that A must be positive and all entries of A must be nonnegative reals.

Now suppose $\mathbf{v}_1, \dots, \mathbf{v}_n$ are vectors satisfying $\langle \mathbf{v}_k, \mathbf{v}_l \rangle \geq 0$, and consider their Gram matrix A ; that is, the $n \times n$ matrix whose k, l -th entry is $\langle \mathbf{v}_k, \mathbf{v}_l \rangle$. Then A is positive and has only nonnegative reals as its entries. So assume A has a positive factorization: $A = B^T B$ for some $m \times n$ matrix B with only nonnegative real entries. Then a trivial check shows that the map

$$\mathbf{v}_k \mapsto \text{the } k^{\text{th}} \text{ column vector of } B \tag{5}$$

is an (inner product preserving) embedding of our vector configuration into the positive orthant of \mathbb{R}^m , and hence that the configuration can be realized in \mathcal{C}_m . By the same argument it is also clear that the Gram matrix of a vector configuration has a positive

factorization if and only if the given configuration can be embedded in the positive orthant of \mathbb{R}^m for some $m \in \mathbb{N}$. Note that it is long known [7, 8, 9, 10, 11] that an $n \times n$ matrix A with only nonnegative entries always has a positive factorization if $n < 5$, and that for $n \geq 5$, as counterexamples show, the same assertion fails.

However, even if the Gram matrix of a given vector configuration does not have a positive factorization, the configuration might still be embeddable into \mathcal{C}_d . In fact, in the next section we shall give a construction showing that if there exists a vector \mathbf{w} such that the angle between \mathbf{w} and \mathbf{v}_k is $\leq \pi/4$ for all $k = 1, \dots, n$, then the configuration $\mathbf{v}_1, \dots, \mathbf{v}_n$ can be embedded in \mathcal{C}_d where $d = 2^{\lfloor n/2 \rfloor}$. In general though, as we shall prove, such a configuration cannot be realized in a positive orthant. By an earlier remark this implies that in general such a configuration — though it can be realized by positive matrices — cannot be realized by *commuting* positive matrices. In fact, our embedding construction relies on the Clifford algebra, which is non-commutative.

Our results, in some sense, can be considered as first examples. Finding a suitable characterization of the configurations that can be realized by positive matrices remains an open problem.

2 Embeddings via the Clifford algebra

In this section we assume (without loss of generality) that the vectors to be represented by positive matrices are given in \mathbb{R}^n . We prove representability if the vectors are contained in the spherical cone

$$C_n = \{\mathbf{v} = (x_1, \dots, x_n) \in \mathbb{R}^n \mid x_1^2 \geq x_2^2 + \dots + x_n^2\}$$

formed by vectors whose angle with the vector $(1, 0, \dots, 0)$ does not exceed $\pi/4$.

Theorem 2.1. *Let $d = 2^{\lfloor n/2 \rfloor}$. There exists an isometric real linear embedding ϕ of \mathbb{R}^n into the space of $d \times d$ self-adjoint complex matrices that maps C_n into the cone \mathcal{C}_d of positive matrices.*

Proof. First assume that $n = 2k + 1$ is odd. Then $d = 2^k$. We identify

$$\mathbb{R}^n = \mathbb{R} \oplus \mathbb{R}^k \oplus \mathbb{R}^k$$

and

$$M_d(\mathbb{C}) = \text{End}_{\mathbb{C}} \left(\bigwedge \mathbb{C}^k \right) = \mathbb{C} \otimes \text{End}_{\mathbb{R}} \left(\bigwedge \mathbb{R}^k \right),$$

where the space of anti-symmetric tensors is endowed with the inner product

$$\left\langle \bigwedge \mathbf{v}_i, \bigwedge \mathbf{w}_j \right\rangle = \det(\langle \mathbf{v}_i, \mathbf{w}_j \rangle).$$

When $\mathbf{v} \in \mathbb{R}^k$, we write $\epsilon_{\mathbf{v}} \in \text{End}(\bigwedge \mathbb{R}^k)$ for the map $\mathbf{u} \mapsto \mathbf{v} \wedge \mathbf{u}$, where \mathbf{u} is any anti-symmetric tensor. We use the anticommutator notation $\{a, b\} = ab + ba$. It is well known that

$$\text{Tr } \epsilon_{\mathbf{v}} = \text{Tr } \epsilon_{\mathbf{v}}^* = 0,$$

$$\{\epsilon_{\mathbf{v}}, \epsilon_{\mathbf{w}}\} = \{\epsilon_{\mathbf{v}}^*, \epsilon_{\mathbf{w}}^*\} = 0$$

and

$$\{\epsilon_{\mathbf{v}}, \epsilon_{\mathbf{w}}^*\} = \langle \mathbf{v}, \mathbf{w} \rangle I.$$

We define

$$\phi : c \oplus \mathbf{v} \oplus \mathbf{w} \mapsto cI + \epsilon_{\mathbf{v}} + \epsilon_{\mathbf{v}}^* + \sqrt{-1}(\epsilon_{\mathbf{w}} - \epsilon_{\mathbf{w}}^*).$$

This clearly maps \mathbb{R}^n to self-adjoint matrices in a linear way. Using the above anticommutation relations, we have

$$\phi(c \oplus \mathbf{v} \oplus \mathbf{w})^2 = c^2 I + \langle \mathbf{v}, \mathbf{v} \rangle I + \langle \mathbf{w}, \mathbf{w} \rangle I + 2c (\epsilon_{\mathbf{v}} + \epsilon_{\mathbf{v}}^* + \sqrt{-1}(\epsilon_{\mathbf{w}} - \epsilon_{\mathbf{w}}^*)).$$

We deduce that ϕ is an isometry since

$$\begin{aligned} |\phi(c \oplus \mathbf{v} \oplus \mathbf{w})|^2 &= \frac{1}{d} \text{Tr} (\phi(c \oplus \mathbf{v} \oplus \mathbf{w})^2) = \\ &= \frac{1}{d} \text{Tr} (c^2 I + \langle \mathbf{v}, \mathbf{v} \rangle I + \langle \mathbf{w}, \mathbf{w} \rangle I) = |c \oplus \mathbf{v} \oplus \mathbf{w}|^2. \end{aligned}$$

Now assume that $c \oplus \mathbf{v} \oplus \mathbf{w} \in C_n$, i.e., $c^2 \geq |\mathbf{v}|^2 + |\mathbf{w}|^2$. We have

$$\phi(c \oplus \mathbf{v} \oplus \mathbf{w}) = cI + \phi(0 \oplus \mathbf{v} \oplus \mathbf{w}).$$

Here the last term is a self-adjoint matrix that squares to $(|\mathbf{v}|^2 + |\mathbf{w}|^2) I$, so its operator norm equals its Euclidean norm, both being the common absolute value of all its eigenvalues, namely $\sqrt{|\mathbf{v}|^2 + |\mathbf{w}|^2} \leq c$. Thus, $\phi(c \oplus \mathbf{v} \oplus \mathbf{w})$ is a positive matrix, which finishes the proof for n odd.

Now assume that $n = 2k$ is even. We still have $d = 2^k$, and there is an obvious isometric embedding $\mathbb{R}^n \rightarrow \mathbb{R}^n \oplus \mathbb{R} = \mathbb{R}^{n+1}$ that maps C_n into C_{n+1} , so the problem is reduced to the odd-dimensional case. \square

As a contrast, we shall now construct a configuration of six vectors in the circular cone $C_3 \subset \mathbb{R}^3$ that cannot be isometrically embedded into the positive orthant $\mathbb{R}_{\geq 0}^d$ for any d .

Put

$$\mathbf{v}_k = \left(1, \cos \frac{2\pi k}{6}, \sin \frac{2\pi k}{6} \right) \in C_3 \subset \mathbb{R}^3 \quad (k \in \mathbb{Z}/6\mathbb{Z}).$$

Theorem 2.2. *It is impossible to have positive vectors $\mathbf{a}_0, \dots, \mathbf{a}_5 \in \mathbb{R}_{\geq 0}^d$ with*

$$\langle \mathbf{a}_j, \mathbf{a}_k \rangle = \langle \mathbf{v}_j, \mathbf{v}_k \rangle \text{ for all } j, k \in \mathbb{Z}/6\mathbb{Z}. \quad (6)$$

Proof. By contradiction, suppose that the positive vectors $\mathbf{a}_0, \dots, \mathbf{a}_5 \in \mathbb{R}_{\geq 0}^d$ satisfy (6).

Put

$$\mathbf{e} = \frac{\mathbf{a}_k + \mathbf{a}_{k+3}}{2};$$

this is independent of k because the analogous statement holds for the \mathbf{v}_k . Put

$$\mathbf{b}_k = \mathbf{a}_k - \mathbf{e} = \mathbf{e} - \mathbf{a}_{k+3}.$$

Then $|\mathbf{b}_k| = |\mathbf{e}|$ and $\mathbf{e} \pm \mathbf{b}_k \in \mathbb{R}_{\geq 0}^d$, so $\mathbf{b}_k = \mathbf{s}_k \circ \mathbf{e}$ (coordinatewise product) for a suitable vector of signs $\mathbf{s}_k \in \{-1, 1\}^d$. But $\mathbf{b}_0 + \mathbf{b}_2 + \mathbf{b}_4 = \mathbf{0}$, so $(\mathbf{s}_0 + \mathbf{s}_2 + \mathbf{s}_4) \circ \mathbf{e} = \mathbf{0}$, which is impossible because every coordinate of $\mathbf{s}_0 + \mathbf{s}_2 + \mathbf{s}_4$ is an odd integer and $\mathbf{e} \neq \mathbf{0}$. \square

3 A configuration which cannot be realized

Put

$$\mathbf{v}_k = \left(\sqrt{\cos \frac{\pi}{5}}, \cos \frac{2\pi k}{5}, \sin \frac{2\pi k}{5} \right) \in \mathbb{R}^3 \quad (k \in \mathbb{Z}/5\mathbb{Z}).$$

Observe that

$$\langle \mathbf{v}_k, \mathbf{v}_{k+1} \rangle = \cos(\pi/5) + \cos(2\pi/5) > 0$$

and

$$\langle \mathbf{v}_k, \mathbf{v}_{k+2} \rangle = \cos(\pi/5) + \cos(4\pi/5) = 0,$$

so $\langle \mathbf{v}_j, \mathbf{v}_k \rangle \geq 0$ for all $j, k \in \mathbb{Z}/5\mathbb{Z}$.

Let \mathcal{M} be a von Neumann algebra with a fixed faithful trace $\tau : \mathcal{M} \rightarrow \mathbb{C}$. (The simplest example is $\mathcal{M} = M_d(\mathbb{C})$ with τ being (a constant multiple of) the ordinary trace.)

Theorem 3.1. *It is impossible to have positive elements $A_0, \dots, A_4 \in \mathcal{M}$ with*

$$\tau(A_j A_k) = \langle \mathbf{v}_j, \mathbf{v}_k \rangle \text{ for all } j, k \in \mathbb{Z}/5\mathbb{Z}. \quad (7)$$

Proof. By contradiction, suppose that the positive elements $A_0, \dots, A_4 \in \mathcal{M}$ satisfy (7). Then

$$\tau(\sqrt{A_k} A_{k\pm 2} \sqrt{A_k}) = \tau(A_k A_{k\pm 2}) = \langle \mathbf{v}_k, \mathbf{v}_{k\pm 2} \rangle = 0,$$

but

$$\sqrt{A_k} A_{k\pm 2} \sqrt{A_k} = \sqrt{A_k} \sqrt{A_{k\pm 2}} \left(\sqrt{A_k} \sqrt{A_{k\pm 2}} \right)^*$$

is positive, so it is zero (since τ is faithful). Thus, $\sqrt{A_k} \sqrt{A_{k\pm 2}} = 0$ and so

$$A_k A_{k\pm 2} = \sqrt{A_k} \sqrt{A_k} \sqrt{A_{k\pm 2}} \sqrt{A_{k\pm 2}} = 0.$$

Now observe that $\mathbf{v}_k, \mathbf{v}_{k+2}$ and \mathbf{v}_{k-2} form a basis of \mathbb{R}^3 , in particular, we have

$$\mathbf{v}_{k\pm 1} \in \mathbb{R}\mathbf{v}_k + \mathbb{R}\mathbf{v}_{k+2} + \mathbb{R}\mathbf{v}_{k-2}.$$

Since the mapping $v_k \mapsto A_k$ preserves inner products, it follows that

$$A_{k\pm 1} \in \mathbb{R}A_k + \mathbb{R}A_{k+2} + \mathbb{R}A_{k-2}.$$

Multiplying on either side by A_k , we get that

$$0 \neq A_k A_{k\pm 1} = A_{k\pm 1} A_k \in \mathbb{R}A_k^2.$$

Note that the product here is nonzero because its trace is strictly positive. We deduce

$$\mathbb{R}A_0^2 = \mathbb{R}A_1 A_0 = \mathbb{R}A_1^2,$$

but the A_k are positive, and the positive square root of a positive operator is unique, so this implies $\mathbb{R}A_0 = \mathbb{R}A_1$. We have an isometry $\mathbf{v}_k \mapsto A_k$, so then $\mathbb{R}\mathbf{v}_0 = \mathbb{R}\mathbf{v}_1$, a contradiction. \square

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