Counting Simplexes in $\mathbb{R}^3$

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Submitted: September 26, 1997; Accepted: January 22, 1998.
AMS Subject Classification: 05D99, 05B35.

Abstract

A finite set of vectors $\mathcal{S} \subseteq \mathbb{R}^n$ is called a *simplex* iff $\mathcal{S}$ is linearly dependent but all its proper subsets are independent. This concept arises in particular from stoichiometry.

We are interested in this paper in the number of simplexes contained in some $\mathcal{H} \subseteq \mathbb{R}^n$, which we denote by $simp(\mathcal{H})$. This investigation is particularly interesting for $\mathcal{H}$ spanning $\mathbb{R}^n$ and containing no collinear vectors.

Our main result shows that for any $\mathcal{H} \subseteq \mathbb{R}^3$ of fixed size not equal to 3, 4 or 7 and such that $\mathcal{H}$ spans $\mathbb{R}^3$ and contains **no** collinear vectors, $simp(\mathcal{H})$ is minimal if and only if $\mathcal{H}$ is contained in two planes intersecting in $\mathcal{H}$, and one of which is of size exactly 3. The minimal configurations for $|\mathcal{H}| = 3, 4, 7$ are also completely described.

The general problem for $\mathbb{R}^n$ remains open.

*The research of the first author was partially supported by NSERC of Canada.
†The research of the second author was partially supported by the Fund "Peregrinatio I" of MOL Co. Hungary, Grant no. 3/1994.

1 Introduction

Simplexes are used for example in stoichiometry when finding minimal reactions and mechanisms, or for finding dimensionless groups in dimensional analysis (see [3]).
To explain the notion of minimal reaction, let the chemical species $A_1, A_2, \ldots, A_n$ consist of elements $E_1, E_2, \ldots, E_m$ as $A_j = \sum_{i=1}^m a_{i,j} E_i$, ($a_{i,j} \in \mathbb{N}$) for $j = 1, 2, \ldots, n$. Writing $\underline{A}_j$ for the vector $[a_{1,j}, a_{2,j}, \ldots, a_{m,j}]^T$, we know that there (might) exists a chemical reaction between the species $\{A_j : j \in S\}$ for any $S \subseteq \{1, 2, \ldots, n\}$ if and only if the homogeneous linear equation

$$\sum_{j \in S} x_j \underline{A}_j = \underline{0} \tag{1}$$

has a non trivial solution for some $x_j \in \mathbb{Z}$, $j \in S$; that is if the vector set $\{\underline{A}_j : j \in S\}$ is *linearly dependent*. Further, the reaction is called **minimal** if for no $T \subsetneq S$ might there be any reaction among the species $\{A_j : j \in T\}$; that is if the vector set $\{\underline{A}_j : j \in T\}$ is *linearly independent* for any $T \subsetneq S$. Of course the reactions obtained in the above way are only possibilities, e.g. the reaction

$$2\mathrm{Au} + 6\mathrm{HCl} \ \rightarrow 2\mathrm{AuCl}_3 + 3\mathrm{H}_2$$

does not occur under normal conditions.

As a specific example, the species A_1 =C, A_2 =O, A_3=CO and A_4=CO_2 determine the vectors $\underline{A}_1 = [1,0], \underline{A}_2 = [0,1], \underline{A}_3 = [1,1]$ and $\underline{A}_4 = [1,2]$, using the "base" {C,O} in $\mathbb{R}^2$. The vector set $H = \{\underline{A}_1, \underline{A}_2, \underline{A}_3, \underline{A}_4\}$ contains the simplexes

$$\{\underline{A}_1, \underline{A}_2, \underline{A}_3\}, \{\underline{A}_1, \underline{A}_2, \underline{A}_4\}, \{\underline{A}_1, \underline{A}_3, \underline{A}_4\} \text{ and } \{\underline{A}_2, \underline{A}_3, \underline{A}_4\}.$$

After solving the corresponding equations (1), we have the following (complete) list of minimal reactions: C+O=CO, C+2O=CO_2, O+CO=CO_2 and C+CO_2=2CO.
We can build up (minimal) **mechanisms** from the above reactions in similar way, which also have important applications (see e.g. [4]).

The investigation can be done without any harm over $\mathbb{R}$ instead of $\mathbb{Z}$, and we arrive at the following abstract definition of a simplex.

Definition 1.1 *A collection $\mathcal{S} \subseteq \mathbb{R}^n$ is called a* **simplex** *if $\mathcal{S}$ is linearly dependent but every proper subset is linearly independent. A k-simplex denotes a simplex of size k.*

In [1], we described which subsets of $\mathbb{R}^n$ of fixed cardinality contain the largest or smallest number of simplexes, allowing collinear vectors. This problem relates to the potential maximal or minimal number of reactions in a given compound.

The largest number of simplexes is easily obtained by placing all vectors in general position, i.e. any n vectors linearly independent. The minimal number of simplexes was obtained allowing collinear vectors, a somewhat artificial condition from the point of view of stoichiometry which translates to having the same species present in various quantities.

In this short note, we completely describe the more appropriate problem of how to obtain the minimal number of simplexes in $\mathbb{R}^3$, allowing **no** collinear vectors. More precisely, if for $\mathcal{H} \subseteq \mathbb{R}^3$ we denote by $simp(\mathcal{H})$ the number of simplexes contained in $\mathcal{H}$, we have:

Theorem 1.2 *For any $\mathcal{H} \subseteq \mathbb{R}^3$ of fixed size not equal to 3, 4 or 7 such that $\mathcal{H}$ spans $\mathbb{R}^3$ and contains* **no** *collinear vectors, $simp(\mathcal{H})$ is minimal if and only if $\mathcal{H}$ is contained in two planes intersecting in $\mathcal{H}$, one of contains exactly three vectors of $\mathcal{H}$; i.e. precisely when $\mathcal{H}$ contains three linearly independent vectors $\{u_1, u_2, u_3\}$, another vector v coplanar with u_1 and u_2 and the rest $\mathcal{H} \setminus \{u_1, u_2, u_3, v\}$ coplanar with u_2 and u_3.*

For $|\mathcal{H}| = 3$, $\mathcal{H}$ must consist of three linearly independent vectors as it is required to span $\mathbb{R}^3$, and therefore $simp(\mathcal{H}) = 0$. For $|\mathcal{H}| = 4$, there are two optimal configurations with 1 simplex. Here and for all subsequent figures, points represent vectors, and aligned points represent vectors in the same plane.

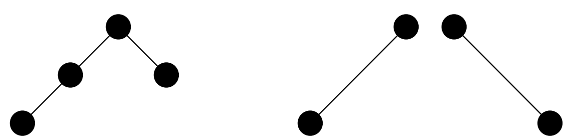

Figure 1: Two optimal configurations for $|\mathcal{H}| = 4$.

For $|\mathcal{H}| = 7$, the analysis contained in this paper will provide the required tools for the reader to verify that there are three optimal configurations with 17 simplexes, one of which is contained in 6 planes each of size 3:

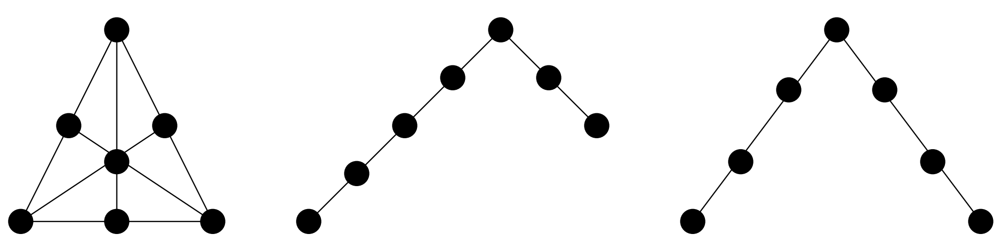

Figure 2: Three optimal configurations for $|\mathcal{H}| = 7$.

Corollary 1.3 *Let $\mathcal{H} \subseteq \mathbb{R}^3$ such that $\mathcal{H}$ spans $\mathbb{R}^3$, $|\mathcal{H}| = m \geq 4$ and contains no collinear vectors. Then we have:*

$$\binom{m-2}{3} + 1 + \binom{m-3}{2} \leq simp(\mathcal{H}) \leq \binom{m}{4}.$$

2 Lower bound in $\mathbb{R}^3$ without collinear vectors

Let $\mathcal{H} \subseteq \mathbb{R}^3$ spanning $\mathbb{R}^3$ but not containing any collinear vectors, which we decompose as

$$\mathcal{H} = \mathcal{P}_1 \cup \mathcal{P}_2 \cup \cdots \cup \mathcal{P}_k \cup \mathcal{I},$$

where the $\mathcal{P}_i$'s constitute the maximal coplanar subsets of $\mathcal{H}$ of size at least 3, which we call *planes*, and $\mathcal{I}$ is the rest, i.e. the vectors of $\mathcal{H}$ not coplanar with two other vectors of $\mathcal{H}$. Letting $p_i = |\mathcal{P}_i|$, we shall always assume that our decompositions is listed so that $p_1 \geq p_2 \geq \cdots \geq p_k \geq 3$.
Notice that in this case, $\mathcal{H} \subseteq \mathbb{R}^3$ not containing any collinear vectors, the only simplexes are 3-simplexes and 4-simplexes, i.e. three coplanar vectors or four vectors no three of which are coplanar. Thus if $|\mathcal{H}| = m$, the number of simplexes of $\mathcal{H}$ can be calculated as

$$simp(\mathcal{H}) = \sum_{i=1}^{k} \binom{p_i}{3} + \binom{m}{4} - \sum_{i=1}^{k} \binom{p_i}{3}(m - p_i) - \sum_{i=1}^{k} \binom{p_i}{4}. \tag{2}$$

We are now ready to undertake the proof of Theorem 1.2. We aim to prove that for $|\mathcal{H}| \neq 3, 4, 7$, we have a unique minimal configuration as described in the theorem, which we denote by $\mathcal{M}_m$, or simply $\mathcal{M}$ when the size is understood.

We first perform a few simplifications.

Lemma 2.1 *The minimal configurations of size ≥ 5 are among those with $\mathcal{I} = \emptyset$.*

Proof: Let $\mathcal{H} \subseteq \mathbb{R}^3$ of size m. If any three vectors of $\mathcal{H}$ are linearly independent, then

$$simp(\mathcal{H}) = \binom{m}{4}.$$

Moving one vector to one coplanar with exactly two others yields $\mathcal{H}'$, still spanning $\mathbb{R}^3$, and

$$simp(\mathcal{H}') = \binom{m-3}{4} + 3\binom{m-3}{3} + 3\binom{m-3}{2} + 1.$$

Therefore

$$simp(\mathcal{H}) - simp(\mathcal{H}') = m - 4 > 0.$$

We can therefore assume that $\mathcal{H}$ contains at least one plane $\mathcal{P}_1$.

If $\mathcal{H} \setminus \mathcal{P}_1$ contains only one vector, then $simp(\mathcal{H}) = \binom{m-1}{3}$, and again

$$simp(\mathcal{H}) - simp(\mathcal{M}) = m - 4 > 0.$$

If now $\mathcal{H} \setminus \mathcal{P}_1$ contains exactly two vectors while $\mathcal{I} \neq \emptyset$, then these two vectors must actually both be in $\mathcal{I}$ and a calculation gives

$$simp(\mathcal{H}) = \binom{m-2}{3} + \binom{m-2}{2} = \binom{m-1}{3}.$$

Moving one of vector of $\mathcal{P}_1$ within the plane to become coplanar with these two vectors results in our optimal configuration $\mathcal{M}$, and a simple calculation gives once again

$$simp(\mathcal{H}) - simp(\mathcal{M}) = m - 4 > 0.$$

Finally assume that $\mathcal{H} \setminus \mathcal{P}_1$ contains at least three vectors, one of these, say u, belonging to $\mathcal{I}$. Form $\mathcal{H}'$ by replacing the vector u by a new vector u' in the plane $\mathcal{P}_1$, not coplanar with any other two vectors of $\mathcal{H} \setminus \mathcal{P}_1$. Then, as $m \geq p_1 + 3$ and $m \geq 5$, we have

$$\begin{aligned} simp(\mathcal{H}) - simp(\mathcal{H}') &= \binom{p_1}{3} - \binom{p_1+1}{3} - \binom{p_1}{3}(m-p_1) \\ &\quad + \binom{p_1+1}{3}(m-p_1-1) - \binom{p_1}{4} + \binom{p_1+1}{4} \\ &\geq \binom{p_1}{2}(m-p_1-2) > 0. \end{aligned}$$

□

Before handling the general case, we settle the situation where $\mathcal{H}$ is contained in exactly two planes.

Lemma 2.2 *For all collections $\mathcal{H} \subseteq \mathbb{R}^3$, $|\mathcal{H}| \neq 7$, contained in two planes, that is $\mathcal{H} = \mathcal{P}_1 \cup \mathcal{P}_2$, $simp(\mathcal{H})$ is minimal exactly when the two planes intersect (in $\mathcal{H}$) and $\mathcal{H}$ has exactly three vectors in one of the planes.*

Proof: Let $\mathcal{H} = \mathcal{P}_1 \cup \mathcal{P}_2$ with $p_1 \geq p_2 \geq 3$. If the two planes do not intersect, form $\mathcal{H}'$ by moving one vector of $\mathcal{P}_2$ to the intersection. Then

$$simp(\mathcal{H}) = \binom{p_1}{3} + \binom{p_2}{3} + \binom{p_1}{2}\binom{p_2}{2},$$

and

$$simp(\mathcal{H}') = \binom{p_1+1}{3} + \binom{p_2}{3} + \binom{p_1}{2}\binom{p_2-1}{2}.$$

Thus $simp(\mathcal{H}) - simp(\mathcal{H}') = \frac{1}{2}p_1(p_1(p_2-2) - p_2) + p_1 > 0$ as $p_1 \geq p_2 \geq 3$.

So we can assume that $\mathcal{H} = \mathcal{P}_1 \cup \mathcal{P}_2$ with $\mathcal{P}_1$ intersecting $\mathcal{P}_2$ in $\mathcal{H}$. Put $p = |\mathcal{P}_2|$ and $|\mathcal{P}_1| = p + q$ for some $q \geq 0$; thus $|\mathcal{H}| = 2p + q - 1$. We compare $simp(\mathcal{H})$ with our optimal configuration $\mathcal{M}$ of size m.

$$simp(\mathcal{H}) = \binom{p+q}{3} + \binom{p}{3} + \binom{p+q-1}{2}\binom{p-1}{2},$$

$$simp(\mathcal{M}) = \binom{2p+q-3}{3} + 1 + \binom{2p+q-4}{2}.$$

Therefore

$$simp(\mathcal{H}) - simp(\mathcal{M}) = \frac{q^2}{4}[(p-3)(p-2)] + \frac{q}{4}[(p-3)(2p^2-9p+6)] + \frac{p}{4}[(p-4)(p-3)^2]$$

and hence $simp(\mathcal{H}) - simp(\mathcal{M}) > 0$ for $p \geq 5$. For $p = 4$, the above formula becomes $\frac{q}{2}(q+1)$ strictly positive for $q > 0$, i.e. $|\mathcal{H}| > 7$; for $|\mathcal{H}| = 7$, there are indeed two optimal configurations of the given form, which are shown on the right hand side of Figure 2. In the case $p = 3$, $\mathcal{H}$ is already in the minimal configuration so there is no change. □

A final preparation shows that one of the planes must have size at least four.

Lemma 2.3 *For all configurations of the form*

$$\mathcal{H} = \mathcal{P}_1 \cup \mathcal{P}_2 \cup \cdots \cup \mathcal{P}_k,$$

where $k \geq 3$ and $|\mathcal{H}| \neq 7$, the optimal ones are among those with $|P_1| \geq 4$.

Proof: Suppose that all planes are of size 3. Then the formula (2) becomes:

$$\begin{aligned} simp(\mathcal{H}) &= \sum_{i=1}^{k}\binom{p_i}{3} + \binom{m}{4} - \sum_{i=1}^{k}\binom{p_i}{3}(m-p_i) - \sum_{i=1}^{k}\binom{p_i}{4} \\ &= k + \binom{m}{4} - 0 - \sum_{i=1}^{k}(m-3) \\ &= \binom{m}{4} - k(m-4). \end{aligned}$$

However $k \leq \binom{m}{2}/3$ and therefore

$$simp(\mathcal{H}) \geq \binom{m}{4} - \binom{m}{2}(m-4)/3.$$

A direct calculation versus our minimal configuration $\mathcal{M}$ gives:

$$\begin{aligned} simp(\mathcal{H}) - simp(\mathcal{M}) &\geq \binom{m}{4} - \binom{m}{2}(m-4)/3 - \binom{m-2}{3} - 1 - \binom{m-3}{2} \\ &= \frac{1}{24}(m^4 - 14m^3 + 55m^2 - 42m - 72) \\ &= \frac{1}{24}(m-3)(m-4)(m^2 - 7m - 6), \end{aligned}$$

which is strictly positive for $m \geq 8$.
The cases $m = 5, 6$ are easily handled separately and 7 is an exception, where a minimal configuration exists with 6 planes each of size 3 (see Figure 2). □

Now we are ready for the final piece.

Lemma 2.4 *For all configurations of the form*

$$\mathcal{H} = \mathcal{P}_1 \cup \mathcal{P}_2 \cup \cdots \cup \mathcal{P}_k,$$

the optimal ones are among those with $k = 2$, unless $|\mathcal{H}| = 7$.

Proof: Recall that $\mathcal{H}$ is required to span $\mathbb{R}^3$ and thus we must have $k \geq 2$; the above configuration also forces $|\mathcal{H}| \geq 5$.
Let $m = |\mathcal{H}|$, and assume that $k \geq 3$. As before, the number of simplexes in $\mathcal{H}$, $simp(\mathcal{H})$, is given by the formula (2) above. By Lemma 2.3, we may assume that $p_1 = |\mathcal{P}_1| \geq 4$.
Form $\mathcal{H}'$ by replacing every vector of $\mathcal{H} \setminus (\mathcal{P}_1 \cup \mathcal{P}_2)$ by new vectors in $\mathcal{P}_2$; also, if the two planes $\mathcal{P}_1$ and $\mathcal{P}_2$ do not already intersect, then replace one of the vectors from $\mathcal{P}_1$ with one in this intersection. Clearly $|\mathcal{H}'| = |\mathcal{H}|$, and as $\mathcal{H}'$ is the union of only two planes, formula (2) becomes:

$$\begin{aligned} simp(\mathcal{H}') &= \binom{p_1}{3} + \binom{m-p_1+1}{3} + \binom{m}{4} - \binom{p_1}{4} \\ &\quad - \binom{m-p_1+1}{4} - \binom{p_1}{3}(m-p_1) - \binom{m-p_1+1}{3}(p_1-1). \end{aligned}$$

Therefore, using (2) again for $simp(\mathcal{H})$, we obtain:

$$\begin{aligned} &simp(\mathcal{H}) - simp(\mathcal{H}') \\ &= \binom{m-p_1+1}{4} + \binom{m-p_1+1}{3}(p_1-2) - \sum_{i=2}^{k}\binom{p_i}{4} - \sum_{i=2}^{k}\binom{p_i}{3}(m-p_i-1). \end{aligned}$$

Hence $simp(\mathcal{H}') \leq simp(\mathcal{H})$ precisely when

$$\sum_{i=2}^{k}\binom{p_i}{4} + \sum_{i=2}^{k}\binom{p_i}{3}(m-p_i-1) \leq \binom{m-p_1+1}{4} + \binom{m-p_1+1}{3}(p_1-2).$$

One difficulty is that m is not well defined in terms of the $p_i s$, and out attempts to prove the inequality directly (under our given conditions) have failed. Instead, we essentially proceed by brute force in defining sets of the appropriate cardinalities and exhibit a 1-1 map from the sets corresponding to the left hand side to the sets corresponding to the right hand side; the slight subtlety comes from also using the structure of these sets to define the map.
Fix two vectors $a, b \in \mathcal{P}_1 \setminus \mathcal{P}_2$ and then choose:

- $\mathcal{P}_i$ itself, as a set of cardinality p_i, for $i = 1, \ldots, k$,
- $\mathcal{P}_1 \setminus \{a, b\}$ as a set of cardinality $p_1 - 2$,
- $(\mathcal{H} \setminus \mathcal{P}_1) \cup \{b\}$ as a set of cardinality $m - p_1 + 1$,
- for $i \geq 2$, define
  $\mathcal{H}_i := \mathcal{H} \setminus (\mathcal{P}_i \cup \{a\})$, if $a \notin \mathcal{P}_i$, or
  $\mathcal{H}_i := \mathcal{H} \setminus (\mathcal{P}_i \cup \{b\})$ if $a \in \mathcal{P}_i$
  as a set of cardinality $m - p_i - 1$.

For a set $\mathcal{X}$ such as $\mathcal{P}_i$, $\mathcal{H}$ or others, we use $\binom{\mathcal{X}}{\ell}$ to denote the collection of ℓ-element subsets of $\mathcal{X}$, a set of size $\binom{|\mathcal{X}|}{\ell}$. Therefore it suffices to define a 1-1 map

$$\bigcup_{i=2}^{k} \binom{\mathcal{P}_i}{4} \cup \bigcup_{i=2}^{k} \binom{\mathcal{P}_i}{3} \times (\mathcal{H}_i) \to \binom{(\mathcal{H} \setminus \mathcal{P}_1) \cup \{b\}}{4} + \binom{(\mathcal{H} \setminus \mathcal{P}_1) \cup \{b\}}{3} \times (\mathcal{P}_1 \setminus \{a, b\}).$$

We proceed in several cases.

A: Let $\mathcal{V} = \{v_1, v_2, v_3, v_4\} \in \bigcup_{i=2}^{k} \binom{\mathcal{P}_i}{4}$.

A1: If $\mathcal{V} \subseteq \mathcal{P}_i$ and $\mathcal{V} \cap \mathcal{P}_1 = \emptyset$, then define
$\mathcal{V} \longmapsto \mathcal{V} \in \binom{(\mathcal{H}\setminus\mathcal{P}_1)\cup\{b\}}{4}$.

A2: If $\mathcal{V} \subseteq \mathcal{P}_i$ and $\mathcal{V} \cap \mathcal{P}_1 \neq \emptyset$, say $v_4 \in \mathcal{V} \cap \mathcal{P}_1$, then

A2.1: if $v_4 \notin \{a, b\}$, define
$\mathcal{V} \longmapsto \mathcal{V} = (\{v_1, v_2, v_3\}, v_4) \in \binom{(\mathcal{H}\setminus\mathcal{P}_1)\cup\{b\}}{3} \times (\mathcal{P}_1 \setminus \{a, b\})$;

A2.2: if $v_4 = b$, define
$\mathcal{V} \longmapsto \mathcal{V} \in \binom{(\mathcal{H}\setminus\mathcal{P}_1)\cup\{b\}}{4}$;

A2.3: if $v_4 = a$, define
$\mathcal{V} \longmapsto \{v_1, v_2, v_3, b\} \in \binom{(\mathcal{H}\setminus\mathcal{P}_1)\cup\{b\}}{4}$.

B: Let $((\mathcal{V}, w) = \{v_1, v_2, v_3\}, w) \in \binom{\mathcal{P}_i}{3} \times \mathcal{H}_i$, $i \geq 2$.

B1: If $\mathcal{V} \cap \mathcal{P}_1 = \emptyset$ and $w \notin \mathcal{P}_1$, the define
$(\mathcal{V}, w) \longmapsto \{v_1, v_2, v_3, w\} \in \binom{(\mathcal{H}\setminus\mathcal{P}_1)\cup\{b\}}{4}$.

B2: If $\mathcal{V} \cap \mathcal{P}_1 = \emptyset$ and $w \in \mathcal{P}_1$, then

B2.1: if $w \notin \{a, b\}$, define
$(\mathcal{V}, w) \longmapsto (\mathcal{V}, w) \in \binom{(\mathcal{H}\setminus\mathcal{P}_1)\cup\{b\}}{3} \times (\mathcal{P}_1 \setminus \{a, b\})$;

B2.2: if $w = b$, then (as $a \notin \mathcal{P}_i$) define
$(\mathcal{V}, w) \longmapsto \{v_1, v_2, v_3, w\} \in \binom{(\mathcal{H}\setminus\mathcal{P}_1)\cup\{b\}}{4}$;

B2.3: Finally $w = a$ is impossible since by construction $a \notin \mathcal{H}_i$.

B3: If $\mathcal{V} \cap \mathcal{P}_1 \neq \emptyset$, say $v_3 \in \mathcal{V} \cap \mathcal{P}_1$, and $w \notin \mathcal{P}_1$, then
B3.1: if $v_3 \notin \{a, b\}$, define
$(\mathcal{V}, w) \longmapsto (\{v_1, v_2, w\}, v_3) \in \binom{(\mathcal{H}\setminus\mathcal{P}_1)\cup\{b\}}{3} \times (\mathcal{P}_1 \setminus \{a, b\})$;
B3.2: if $v_3 = b$, define
$(\mathcal{V}, w) \longmapsto \{v_1, v_2, v_3, w\} \in \binom{(\mathcal{H}\setminus\mathcal{P}_1)\cup\{b\}}{4}$;

B3.3: if $v_3 = a$, then as $|\mathcal{P}_1| \geq 4$, choose $c \in \mathcal{P}_1 \setminus \{a\}$ not coplanar with either w and v_1 or w and v_2. Now define

$$\begin{array}{ll} (\mathcal{V}, w) \longmapsto (\{v_1, v_2, w\}, c) \in \binom{(\mathcal{H}\setminus\mathcal{P}_1)\cup\{b\}}{3} \times (\mathcal{P}_1 \setminus \{a, b\}), & \text{if } c \neq b, \\ (\mathcal{V}, w) \longmapsto \{v_1, v_2, w, b\} \in \binom{(\mathcal{H}\setminus\mathcal{P}_1)\cup\{b\}}{4} & \text{if } c = b. \end{array}$$

B4: If $\mathcal{V} \cap \mathcal{P}_1 \neq \emptyset$, say $v_3 \in \mathcal{V} \cap \mathcal{P}_1$, and $w \in \mathcal{P}_1$, then
B4.1: if $v_3 \notin \{a, b\}$ and $w \notin \{a, b\}$), define
$(\mathcal{V}, w) \longmapsto (\{v_1, v_2, b\}, w) \in \binom{(\mathcal{H}\setminus\mathcal{P}_1)\cup\{b\}}{3} \times (\mathcal{P}_1 \setminus \{a, b\})$;

B4.2: if $v_3 \notin \{a, b\}$, then $w = a$ is impossible since by construction $a \notin \mathcal{H}_i$;

B4.3: if $v_3 \notin \{a, b\}$ and $w = b$, define
$(\mathcal{V}, w) \longmapsto (\{v_1, v_2, b\}, v_3) \in \binom{(\mathcal{H}\setminus\mathcal{P}_1)\cup\{b\}}{3} \times (\mathcal{P}_1 \setminus \{a, b\})$;
B4.4: if $v_3 = a$ (and therefore $w \notin \{a, b\}$), define
$(\mathcal{V}, w) \longmapsto (\{v_1, v_2, b\}, w) \in \binom{(\mathcal{H}\setminus\mathcal{P}_1)\cup\{b\}}{3} \times (\mathcal{P}_1 \setminus \{a, b\})$;
B4.5: if $v_3 = b$ (and therefore $w \notin \{a, b\}$), define
$(\mathcal{V}, w) \longmapsto (\mathcal{V}, w) \in \binom{(\mathcal{H}\setminus\mathcal{P}_1)\cup\{b\}}{3} \times (\mathcal{P}_1 \setminus \{a, b\})$.

One can methodically verify that the above map is 1-1 as in every case the exact preimage is recuperated from the structure of the image.

Indeed, first let (v_1, v_2, v_3, v_4) be a 4-tuple in the range $\binom{(\mathcal{H}\setminus\mathcal{P}_1)\cup\{b\}}{4}$. If b does not appear, then the tuple can only arise from A1 or B1, and in both cases the preimage is the tuple itself or the pair $(\{v_1, v_2, v_3\}, v_4)$. Now assume that b appears, say $v_4 = b$. If all v_i's are coplanar, then it must have been obtained from A2.2, and the preimage is again the tuple itself. On the other hand, if $\{v_1, v_2, v_3\}$ is not coplanar, then the tuple can only have been obtained by B3.3, in which case the preimage is $(\{v_1, v_2, v_3\}, a)$. If $\{v_1, v_2, v_3\}$ is coplanar with a (and therefore $b \notin \mathcal{H}_i$), then the tuple can only have been obtained by A2.3, in which case the preimage is (v_1, v_2, v_3, a). Finally if $v_4 = b \in \mathcal{P}_i$, then we are in case B3.2, else we are in case B2.2, and in both cases the preimage is $(\{v_1, v_2, v_3\}, v_4)$.

Finally consider a pair $(\{v_1, v_2, v_3\}, w)$ in the range $\binom{(\mathcal{H}\setminus\mathcal{P}_1)\cup\{b\}}{3} \times (\mathcal{P}_1 \setminus \{a, b\})$. If w is coplanar with $\{v_1, v_2, v_3\}$, then we are in case A2.1, and the pair came from the 4-tuple (v_1, v_2, v_3, w). If w is coplanar with two of the vectors, say v_1 and v_2, then we must be in either case B3.1 or B4.3, which are settled by whether v_3 belongs to $\mathcal{P}_1$ or not. If it does, which also implies that $v_3 = b$, then we are in case B4.3 and the preimage is $(\{v_1, v_2, w\}, v_3)$. If it does not, then we are in case B3.1 and the preimage is also $(\{v_1, v_2, w\}, v_3)$, but without b appearing. If (say) $v_3 = b$, then we are in either case B4.1, B4.4 or B4.5. If moreover $\{v_1, v_2, v_3\}$ is coplanar, then we must be in case B4.5 and the preimage is the pair $(\{v_1, v_2, v_3\}, w)$ itself. If the plane $\mathcal{P}_i$ spanned by $\{v_1, v_2\}$ intersects the plane $\mathcal{P}_1$ in a, then we are in case B4.4, and the preimage is $(\{v_1, v_2, a\}, w)$. Otherwise, we are in case B4.1, and if $u(\neq a)$ denotes the intersection of the planes $\mathcal{P}_i$ and $\mathcal{P}_1$, then the preimage is $(\{v_1, v_2, u\}, w)$. Now after all this if $\{v_1, v_2, v_3\}$ is coplanar, then we are in case B2.1 and the preimage if the pair itself. The last case is when the plane spanned by two of the vectors, say v_1 and v_2, also contains a. Then we are in case B3.3 and the preimage is $(\{v_1, v_2, a\}, v_3)$.

To conclude the proof of the Lemma, assume that $\mathcal{H} \setminus (\mathcal{P}_1 \cup \mathcal{P}_2) \neq \emptyset$, and consider $\mathcal{H}'$ formed as described above. We have shown that $simp(\mathcal{H}') \leq simp(\mathcal{H})$, but now $\mathcal{H}'$ consists of two planes both of size at least 4; so $simp(\mathcal{H}')$ and a priori $simp(\mathcal{H})$ is not a minimal configuration by Lemma 2.2. This completes the proof. □

We now have all the necessary tools to complete the proof of Theorem 1.2. Consider a collection $\mathcal{H} = \mathcal{P}_1 \cup \cdots \cup \mathcal{P}_k \cup \mathcal{I}$ with $simp(\mathcal{H})$ as small as possible. By Lemma 2.1, we can assume that $\mathcal{I} = \emptyset$ if $|\mathcal{H}| \geq 5$; by Lemma 2.4, we can assume that $k = 2$ if $|\mathcal{H}| \neq 7$. But then Lemma 2.2 uniquely determines $\mathcal{H}$ as our minimal configuration $\mathcal{M}$. The exceptional configurations for $|\mathcal{H}| = 3, 4, 7$ are given in figures 1 and 2. □

3 Conclusion

The general problem in $\mathbb{R}^n$ regarding the minimum size of $simp(\mathcal{H})$ where $\mathcal{H}$ is of fixed size, spans $\mathbb{R}^n$ and contains no collinear vectors remains open. However we conjecture that the minimum is attained precisely for the following configurations.

1 If n is even, $\mathcal{H}$ contains n linearly independent vectors $\{u_i : i = 1, \ldots, n\}$ and the remaining divided as evenly as possible between the planes $\{[u_i, u_{i+1}]; i = 1, 3, \ldots, n-1\}$.

2 If n is odd, $\mathcal{H}$ again contains n linearly independent vectors $\{u_i : i = 1, \ldots, n\}$, one extra vector in the plane $[u_{n-1}, u_n]$ and finally the remaining vectors divided as evenly as possible between the planes $\{[u_i, u_{i+1}]; i = 1, 3, \ldots, n-2\}$ with lower indices having precedence.

The authors are grateful to Professor Árpád Pethő for drawing their attention to this problem, and thank student Jianzhong Meng for his help with some calculations with Maple.

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