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COUNTING SIMPLEXES IN $\Re^n$

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A finite set of vectors $\mathbb{S} \subset \Re^n$ is called a simplex if $\mathbb{S}$ is linearly dependent but all its proper subsets are independent. If we denote the number of simplexes contained in $\mathcal{H} \subseteq \Re^n$ by *simp*($\mathcal{H}$), then our main results can be formulated as:

THEOREM: For any $\mathcal{H} \subseteq \Re^n$ of fixed size, *simp*($\mathcal{H}$) is maximal if any *n* vectors of $\mathcal{H}$ are linearly independent.

THEOREM: For any $\mathcal{H} \subseteq \Re_n$ of fixed size so that $\mathcal{H}$ spans $\Re^n$, *simp*($\mathcal{H}$) is minimal if $\mathcal{H}$ consists of *n* collections of parallel vectors of sizes differing by at most one from each other.

COROLLARY: Let $\mathcal{H} \subseteq \Re^n$ so that $\mathcal{H}$ spans $\Re^n$ and $|\mathcal{H}| = m$. Then writing $m = an + b$ where $0 \le b < n$, we have:

$$b\binom{a+1}{2} + (n-b)\binom{a}{2} \le simp(\mathcal{H}) \le \binom{m}{n+1}.$$

The related problem regarding the minimum value of *simp*($\mathcal{H}$) under the condition that parallel vectors are not allowed in $\mathcal{H}$ remains open.

Introduction

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

Therefore a 2-simplex is just a pair of parallel vectors and in general a *k*+1-simplex is a collection of *k*+1 vectors which span a subspace of dimension *k*.

Simplexes are widely used e.g. in stoichiometry when finding minimal reactions and mechanisms (which have further important applications in chemistry), or for finding dimensionless group in dimensional analysis [2].

Consider the notion of minimal reactions. Let the chemical species $A_1, A_2, ..., A_m$ consist of elements E_1, $E_2, ..., E_n$ as

$$A_j = \sum_{i=1}^{n} a_{i,j} E_i, \ (a_{i,j} \in \mathbb{N}) \text{ for } j = 1, 2, ..., m.$$

Writing $\mathbf{A}_j$ for the vector $[a_{1,j}, a_{2,j}, ..., a_{n,j}]^T$, we know that there (perhaps) exists a chemical reaction between the species $\{A_j : j \in \mathbb{S}\}$ for any $\mathbb{S} \subseteq \{1, 2, ..., m\}$ if and only if the homogeneous linear equation

$$\sum_{j \in \mathbb{S}} x_j \mathbf{A}_j = 0 \qquad (1)$$

has a non trivial solution for some $x_j \in \Re, j \in \mathbb{S}$; that is if the vector set $\{\mathbf{A}_j : j \in \mathbb{S}\}$ is *linearly dependent*. Further, the reaction is called **minimal** if for no $\mathbf{T} \not\subset \mathbb{S}$ might there be any reaction among the species $\{A_j : j \in \mathbf{T}\}$; that is if the vector set $\{\mathbf{A}_j : j \in \mathbf{T}\}$ is *linearly independent* for any $\mathbf{T} \not\subset \mathbb{S}$. Of course the reactions obtained in the above way are only possibilities, e.g. the reaction

$$2\,Au + 6\,HCl \rightarrow 2\,AuCl_3 + 3\,H_2$$

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 $\mathbf{A}_1 = [1, 0]$, $\mathbf{A}_2 = [0, 1]$, $\mathbf{A}_3 = [1, 1]$ and $\mathbf{A}_4 = [1, 2]$, using the "base" {C, O} in $\Re^2$. The vector set $\mathcal{H} = \{A_1, A_2, A_3, A_4\}$ contains the simplexes

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

After solving the corresponding *Eq.(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 a similar way, which also have important applications [3].

For further details and examples see Refs. [1] and [3]. This last reference further provides a computer algorithm for the pure algebraic problem of finding all the simplexes in a given set of vectors in $\mathcal{R}^n$, *without repetition*. In Ref. [1], the author presents a theoretical approach of the problem.

The main question of the present work is:

"How many simplexes (minimum or maximum) can be found in a given set of vectors $\mathcal{H} \subset \mathcal{R}^n$ if n and the size of $\mathcal{H}$ are fixed?"

In other words, we want bounds for simplexes (minimal reactions) whenever the dimension (number of possible atoms) and the size of the given vector set (number of species) are given.

Definition 1.2. For $\mathcal{H} \subseteq \mathcal{R}^n$, we write

$$simp(\mathcal{H}) = |\{ \mathcal{S} \subseteq \mathcal{H} : \mathcal{S} \text{ is a simplex}\}|.$$

In this paper, we explicitly calculate both the possible maximum and minimum values of $simp(\mathcal{H})$ for all $\mathcal{H}$'s of a fixed size. Our main results are the following:

Theorem 1.3. For any $\mathcal{H} \subseteq \mathcal{R}^n$ of fixed size (so that $\mathcal{H}$ spans $\mathcal{R}^n$), $simp(\mathcal{H})$ is maximal if and only if any n vectors of $\mathcal{H}$ are linearly independent.

Theorem 1.4. For any $\mathcal{H} \subseteq \mathcal{R}^n$ of fixed size so that $\mathcal{H}$ spans $\mathcal{R}^n$, $simp(\mathcal{H})$ is minimal if and only if $\mathcal{H}$ consists of n collections of parallel vectors of sizes differing by at most one from each other.

Corollary 1.5. Let $\mathcal{H} \subseteq \mathcal{R}^n$ so that $\mathcal{H}$ spans $\mathcal{R}^n$ and $|\mathcal{H}| = m$. Then, writing $m = an + b$ where $0 \le b < n$, we have:

$$b\binom{a+1}{2} + (n-b)\binom{a}{2} \le simp(\mathcal{H}) \le \binom{m}{n+1}.$$

Unfortunately our methods in the minimum case only work if we allow parallel vectors (i.e. to use the same species more than one time). So lower bound could be much bigger when excluding parallel vectors and this problem remains open. (This restriction is irrelevant in the maximum case.)

However we conjecture that in the case of $\mathcal{R}^3$, the minimum is attained when

$$\mathcal{H} = \{u_1, u_2, u_3\} \cup \{v\} \cup \{w_i : i < m-4\}$$

where $\{u_1, u_2, u_3\}$ are linearly independent, $v \in [u_1, u_2]$, and $\{w_i : i < m\} \subseteq [u_2, u_3]$. Thus we conjecture that the minimal number of simplexes is $\binom{m-2}{3} + 1 + \binom{m-3}{2}$ in this case.

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Upper Bound

Proof of Theorem 1.3: Fix $\mathcal{H} \subseteq \mathcal{R}^n$ of size m. Choose $\mathcal{V} = \{v_1, v_2, ..., v_n\} \subseteq \mathcal{H}$ spanning $\mathcal{R}^n$, and suppose $u \in \mathcal{H} \setminus \mathcal{V}$ belongs to a linearly dependent subset of $\mathcal{H}$ of size at most n. Chose $u' \in \mathcal{R}^n$ not in any subspace generated by any n-1 elements of $\mathcal{H}$. Define now

$$\mathcal{H}' := (\mathcal{H} \setminus \{u\}) \cup \{u'\}$$

Then $|\mathcal{H}'| = |\mathcal{H}|$ and we first show that $simp(\mathcal{H}') \ge simp(\mathcal{H})$.

So let $\mathcal{S} = \{u_1, u_2, ..., u_k\}$ be a simplex of $\mathcal{H}$. If $u \notin \mathcal{S}$ then $\mathcal{S}$ is still a simplex of $\mathcal{H}'$. If u is an element of $\mathcal{S}$, say $u = u_i$, then $\mathcal{S} \setminus \{u_i\}$ is linearly independent, and so we can choose $\mathcal{V}' \subseteq \mathcal{V}$ of size n-k+1 so that $\mathcal{S} \setminus \{u_i\} \cup \mathcal{V}'$ is again linearly independent but also spans $\mathcal{R}^n$. But then $\mathcal{S}' := \mathcal{S} \setminus \{u_i\} \cup \mathcal{V}' \cup \{u'\}$ is a new simplex of $\mathcal{H}'$. Moreover, the map $\mathcal{S} \to \mathcal{S}'$ is one-to-one, and hence $simp(\mathcal{H}') \ge simp(\mathcal{H})$ as desired.

Thus $simp(\mathcal{H})$ is maximal when any n element of $\mathcal{H}$ are linearly independent; we now show that no other configuration may have so many simplexes.

For this, let $\mathcal{S} \subseteq \mathcal{H}$ be a fixed simplex of l element. Using the above construction repeatedly m-l many times, we can assume that no vector u of $\mathcal{H}' \setminus \mathcal{S}$ belongs to any subspace generated by n-1 elements of $\mathcal{H} \setminus \{u\}$.

However it is now easy to obtain an upper bound for the number of simplexes in $\mathcal{H}$; indeed we have $\mathcal{S}$ itself which is preserved and then there are only n+1 element simplexes which must contain at most l-1 elements of $\mathcal{S}$. That is

$$simp(\mathcal{H}) \le 1 + \sum_{i=0}^{l-1} \binom{l}{i}\binom{m-l}{n+1-i} = 1 + \binom{m}{n+1} - \binom{m-l}{n+1-l}$$

But this quantity is strictly less than $\binom{m}{n+1}$ whenever $n + 2 \leq m$. For $m = n$, there are no simplexes and for $m = n + 1$, there is a configuration with exactly one k-simplex for every $2 \leq k \leq n+1$. This completes the proof.

Lower Bound

In this section we give a lower bound for the number of simplexes contained in collection of vectors $\mathcal{H} \subseteq \mathcal{R}^n$ of fixed size. We show that this bound is sharp when we allow parallel vectors in $\mathcal{H}$; namely we provide a construction which attains this minimal number of simplexes for each prescribed size of $\mathcal{H}$. It turns out that, as for the maximal case above, this construction is unique (in terms if the number of linear independent or parallel vectors in $\mathcal{H}$).

Proof of Theorem 1.4. Fix n and m and consider a collection $\mathcal{H} \subseteq \mathcal{R}^n$ of size m which also spans $\mathcal{R}^n$ and for which $simp(\mathcal{H})$ is minimal.

Let $\theta_1, \theta_2, \ldots, \theta_p$ be the distinct collections of parallel vectors of $\mathcal{H}$, and abusing notation, let $\theta_1, \theta_2, \ldots, \theta_p$ be members of each class, which we use as representatives of the classes. We shall also use θ_i to denote $|\theta_i|$, the size of the collection θ_i.

For any set of vectors $\mathcal{S} \subseteq \mathcal{R}^n$, $[\mathcal{S}]$ denotes the *linear hull of* $\mathcal{S}$. We call a simplex *large* if it contains at least 3 elements.

Lemma 3.1. If $\mathcal{H}$ contains a minimal number of simplexes, then all vectors contained in large simplexes are contained in no other simplex; therefore we may assume that $\mathcal{H}$ has no large simplexes.

Proof. Let $\mathcal{H} = \bigcup_{i=1}^{p} \theta_i$ and suppose that $\mathcal{H}$ contains a large simplex $\mathcal{S}$; this forces $p \geq n+1$. By relabeling, we may assume that θ_1 and θ_2 are members of $\mathcal{S}$ and that actually $\mathcal{S} = \{\theta_i : i \in \mathcal{I}\}$. We define:

- k = the number of large simplexes that contain both θ_1 and θ_2,
- k_1 = the number of large simplexes containing θ_1 but not θ_2,
- k_2 = the number of large simplexes containing θ_2 but not θ_1

and suppose without loss of generality that $k_1 \geq k_2$.

Take note that $k \geq \prod_{i \in \mathcal{I} \setminus \{1,2\}} \theta_i$

Now we form $\mathcal{H}'$ by deleting all elements of the collection θ_1 and replacing each of them by a new vector in the collection of θ_2. Observe that $\mathcal{H}'$ still spans $\mathcal{R}^n$, as θ_1 was a linear combination of the other members of any large simplex containing it. Further, this modification only affects the simplexes containing at least one member of θ_1 or θ_2.

Before this modification, $\mathcal{H}$ contained

$$\binom{\theta_1}{2} + k_1\theta_1 + \binom{\theta_2}{2} + k_2\theta_2 + k\theta_1\theta_2$$

many simplexes containing a member of either θ_1 or θ_2.

After this construction, $\mathcal{H}'$ will have

$$\binom{\theta_1+\theta_2}{2} + k_2(\theta_2+\theta_1)$$

of such simplexes. The remaining simplexes are unchanged.

By minimality of $simp(\mathcal{H})$, we must have

$$\binom{\theta_1}{2} + k_1\theta_1 + \binom{\theta_2}{2} + k_2\theta_2 + k\theta_1\theta_2 \leq \binom{\theta_1+\theta_2}{2} + k_2(\theta_2+\theta_1)$$

which, after an elementary calculation, reduces to

$$k_1 - k_2 \leq \theta_2(1-k)$$

and therefore $k = 1$ (as $k \geq 1$) and $k_1 = k_2$. Thus $1 = k \geq \prod_{i \in \mathcal{I} \setminus \{1,2\}} \theta_i$ which forces (by symmetry) that $\theta_i = 1$ for each $i \in \mathcal{I}$.

But now, if a vector v belongs to two different large simplexes $\mathcal{S}_1$ and $\mathcal{S}_2$, then $(\mathcal{S}_1 \cup \mathcal{S}_2) \setminus \{v\}$ is a linearly dependent collection on non-parallel vectors which therefore must contain a large simplex $\mathcal{S}'$. But $\mathcal{S}'$ must contain at least 2 elements from either $\mathcal{S}_1$ or $\mathcal{S}_2$ which contradicts the previous paragraph. This proves the first part of the Lemma.

Finally, without changing $simp(\mathcal{H})$, we may replace one vector of a large simplex $\mathcal{S}$ by one parallel to another member of $\mathcal{S}$ which in effect replaces a large simplex of $\mathcal{H}$ by a 2-simplex. This completes the proof.

Now we turn to vectors contained *only* in "small" simplexes, i.e. in pairs of parallel vectors.

Lemma 3.2. If $|\mathcal{H}| = m$ and $simp(\mathcal{H})$ is minimal, then all vectors must belong to a collection of parallel vectors of sizes differing by at most 1.

Proof. By Lemma 3.1, we can assume that $\mathcal{H}$ contains no large simplex. Obviously, each collection θ_i of parallel vectors accounts for $\binom{\theta_i}{2}$ such simplexes.

If $\theta_i > \theta_j + 1$, then putting one vector from θ_i to θ_j decreases the number of simplexes in $\mathcal{H}$ as shows the inequality

$$\binom{\theta_i}{2}+\binom{\theta_j}{2}>\binom{\theta_i-1}{2}+\binom{\theta_j+1}{2}$$

This completes the proof.

These Lemmas essentially prove Theorem 1.4. Indeed, given a collection $\mathcal{H} \subseteq \mathcal{R}^n$ of size m which spans $\mathcal{R}^n$ and for which $simp(\mathcal{H})$ is minimal, we can write

$$\mathcal{H}=\bigcup_{i=1}^{n}\theta_i$$

and therefore, if $m = an + b$ where $0 \leq b < n$,

$$simp(\mathcal{H}) = b\binom{a+1}{2}+(n-b)\binom{a}{2} \leq simp(\mathcal{H})$$

as desired. The strict inequality in Lemma 3.2 shows that this configuration is unique.

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