Discrete Applied Mathematics 180 (2015) 141–149

Contents lists available at ScienceDirect

Discrete Applied Mathematics

journal homepage: www.elsevier.com/locate/dam

Minimum number of affine simplices of given dimension

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ARTICLE INFO

Article history:
Received 26 September 2013
Received in revised form 19 July 2014
Accepted 22 July 2014
Available online 12 August 2014

Keywords:
Linear hypergraph
Extremal set theory
Euclidean affine simplex
Minimal linear dependency
Stoichiometry

ABSTRACT

In this paper we formulate and solve extremal problems in the Euclidean space $\mathbb{R}^d$ and further in hypergraphs, originating from problems in stoichiometry and elementary linear algebra. The notion of affine simplex is the bridge between the original problems and the presented extremal theorem on set systems. As a sample corollary, it follows that if no triple is collinear in a set S of n points in $\mathbb{R}^3$, then S contains at least $\binom{n}{4} - cn^3$ affine simplices for some constant c. A function related to Sperner's Theorem and its well-known extension to reciprocal sums is also considered and its relation to Turán's hypergraph problems is discussed.

1. Introduction

The roots of the present study date back to the mid-1980s, to the paper by S. Kumar and Á. Pethő [7], concerning an application of linear algebra in stoichiometry. From the algebraic point of view, their very natural question asks about the number of those subsets of a set of vectors which are linearly dependent but each of whose proper subsets is independent. Here we give an asymptotically tight solution for the minimum in terms of dimension and the number of vectors when low-dimensional dependencies are excluded. Our method is to prove a more general result in extremal set theory (Theorem 6 below), hence without assuming anything about the structure of algebraic dependencies.

1.1. Motivation in chemistry

Restricting attention to a "universe" of D kinds of atoms (or atomic parts), each molecule (species) can be represented with a vector in $\mathbb{R}^D$ whose ith coordinate means the number of atoms of ith type in the molecule in question.[1] Then a chemical reaction naturally corresponds to a zero-sum linear combination of these vectors (using the law of mass balance).

The reaction is called minimal if none of the molecules, taking role in it, can be omitted so that the remaining ones could form still a(nother) reaction. In the language of linear algebra this assumption is equivalent to the property that the corresponding set of vectors is linearly dependent but each proper subset of it is independent, that is the defining condition of *linear algebraic simplex*. Both from practical and theoretical purposes the following problem was raised:

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[1] The types of atoms are supposed to be in a fixed order. E.g., if $D = 3$ and the universe is [C, H, O], then we have the vector $(0, 2, 1)$ for H_2O and $(2, 4, 2)$ for CH_3COOH.

http://dx.doi.org/10.1016/j.dam.2014.07.025
0166-218X/

Problem 1. What is the minimum and maximum number of linear algebraic simplices $S \subseteqq \mathcal{V}$ in a set $\mathcal{V}$ of vectors in $\mathbb{R}^D$ if only the size $|\mathcal{V}|$ is given and $\mathcal{V}$ spans $\mathbb{R}^D$? What are the structures of sets $\mathcal{V}$ which contain extremal number of simplices?

The answer was given in [8]. Moreover, Problem 1 was generalized for matroids in [4]; actually its authors solved it a decade earlier than published, see [3].

Concerning the minimum, the results in [8] show that almost all vectors must be *parallel*, i.e. almost all molecules (species) are isomer molecules or multiple doses. The problem where parallel vectors are excluded is still unsolved in general:

Problem 2. What is the minimum number of linear algebraic simplices $S \subseteqq \mathcal{V}$ if only the size $|\mathcal{V}|$ is given, $\mathcal{V}$ does not contain parallel vectors and $\mathcal{V}$ spans $\mathbb{R}^D$? What are the structures of sets $\mathcal{V}$ which contain the minimum number of simplices?

A conjecture on both the minimum number and the structure attaining it is stated in [9]. The cases $D = 3$ and $D = 4$ were solved in [9,17], respectively.

1.2. Geometric formulation

In the framework of linear algebra the problem is somewhat non-symmetric because the zero vector plays a special role. This asymmetry can be eliminated if we translate the problem to the language of geometry. Moreover, restricting attention to sets $\mathcal{V} \subset \mathbb{R}^D$ containing neither the zero vector nor a pair of parallel vectors, the dimension can be reduced from D to $d = D - 1$: first associate each element $\underline{v} \in \mathcal{V}$ with its direction $\lambda \cdot \underline{v}$ $(\lambda \in \mathbb{R})$, and then intersect this system $\Lambda\mathcal{V}$ with a $(D-1)$-dimensional hyperplane $\mathcal{P}$ which does not contain the origin and is not parallel to any element of $\mathcal{V}$.

The mapping from $\mathcal{V}$ to the set $\mathcal{V}^{\mathcal{P}} := \Lambda\mathcal{V} \cap \mathcal{P}$ is a bijection under which linear algebraic simplices $S \subset \mathcal{V}$ correspond to *affine simplices* $S^{\mathcal{P}} \subset \mathbb{R}^{D-1}$, where a set S of $k \geq 3$ points in the Euclidean d-space is called an *affine simplex* if S is contained in some $(k-2)$-dimensional hyperplane but no proper subset $S' \subsetneqq S$ is contained in a hyperplane of dimension $|S'| - 2$. For instance, in $\mathbb{R}^3$ the following three types of affine simplices occur:

- three collinear points;
- four coplanar points, no three of which are collinear;
- five points, no four of which are coplanar.

Affine simplices can alternatively be defined by requiring that the vectors $\underline{s}_2 - \underline{s}_1, \underline{s}_3 - \underline{s}_1, \ldots, \underline{s}_k - \underline{s}_1$ be linearly dependent but their proper subsets should not (for every choice of a point to be labeled $\underline{s}_1$).

In cases of low dimension, as solved in [9,17], almost all points of the extremal configurations for Problem 2 attaining the minimum number of affine simplices lie on one or two lines, i.e. mostly contain affine simplices of three points. In this way the natural question arises to determine the minimum in the other extreme, where no three points are collinear. For this reason our goal is to study point sets which contain no affine simplices smaller than a given size. The first interesting case is $\mathbb{R}^3$.

Let $S \subset \mathbb{R}^d$ be a set of n points, no d of which lie on a $(d-2)$-dimensional hyperplane. Then two kinds of subsets of S form an affine simplex:

- $d + 1$ points on a hyperplane of dimension $d - 1$, or
- $d + 2$ points, no $d + 1$ of which lie on a common hyperplane of dimension $d - 1$.

Theorem 3. *For every $d \geq 3$ there is a constant $c = c(d)$ with the following property. If $S \subset \mathbb{R}^d$ is a set of n points, no d of them lying on a hyperplane of dimension $d - 2$, then S determines at least $\binom{n}{d+1} - cn^d$ affine simplices.*

Corollary 4. *For any n points in the 3-space, no three being collinear, the number of coplanar quadruples plus the 5-tuples containing no coplanar quadruples is at least $\binom{n}{4} - O(n^3)$ as $n \to \infty$.*

These results are asymptotically tight, as shown by the obvious example of n coplanar points in $\mathbb{R}^3$ (no three of them being on a line) and also for any $d \geq 3$ by n points of $\mathbb{R}^{d-1}$ in general position when embedded isometrically into $\mathbb{R}^d$. Such a set of points has exactly $\binom{n}{d+1}$ affine simplices. In fact, configurations with even fewer affine simplices exist, which in addition span the d-space. For instance, $n-1$ points of $\mathbb{R}^{d-1}$ in general position embedded in a hyperplane of $\mathbb{R}^d$ plus an nth point outside that hyperplane generate just $\binom{n-1}{d+1}$ affine simplices (as no affine simplex contains the nth point).

In $\mathbb{R}^3$, the two arrangements of points just mentioned yield $\frac{1}{24}n^4 - \frac{1}{4}n^3 + O(n^2)$ and $\frac{1}{24}n^4 - \frac{5}{12}n^3 + O(n^2)$, respectively. Currently we do not know whether or not the latter error term $\frac{5}{12}n^3$ is asymptotically tight. We do know, however, that the construction above is not extremal; an improvement of the order $O(n^2)$ will be proved in Proposition 7.

1.3. Combinatorial formulation

Here we put the problems and results above in a more general setting. Let $\mathcal{H} = (X, \mathcal{E})$ be a hypergraph, where X is the finite vertex set and $\mathcal{E}$ is the edge set consisting of subsets of X. We extend the notion of linear hypergraph (also called "simple" or "almost disjoint" in some parts of the literature) as follows.