Reactions, mechanisms and simplexes

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Many thanks to

FIELDS

(1) **Chemical reactions** :

$$2\,H_2 + 2\,CO = CH_4 + CO_2$$

Linear combination

```
H:     |2|      |0|    |4|    |0|    |0|
C:  2*|0| + 2*|1| - |1| - |1| = |0|
O:     |0|      |1|    |0|    |2|    |0|
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<u>Minimal</u>: none of them can be omitted.

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Minimal: none of them can be omitted.

(also for ions, e^-, cathalysts, etc.)

(2) **Mechanisms** :

1:	C + O = CO	$\underline{X}_1$ = [1,1,-1,0]
2:	C + 2 O = CO_2	$\underline{X}_2$ = [1,2,0,-1]
(3:	O + CO = CO_2	$\underline{X}_3$ = [0,1,1,-1])
4:	C + CO_2 = 2CO	$\underline{X}_4$ = [1,0,-2,1]

~~~~~~

$$2*\underline{X}_1 - \underline{X}_2 = \underline{X}_4$$

Linear combination

$$2*\underline{X}_1 - \underline{X}_2 - \underline{X}_4 = \underline{0}$$
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Minimal: none of them can be omitted.

Prescribed: input- , output- materials
~~~~~~

(3) **Physical quantities** (**measure units/**"dimension analysis"**):**

[1, 0, 0, 0, 0, 0]

[0, 1,-1, 0, 0, 0]

[-3, 0, 0, 1, 0, 0]

[-1, 0,-1, 1, 0, 0]

[0, 0,-2, 0, 1,-1]

[0, 0,-3, 1, 0,-1]

[1, 0,-3, 1, 0,-1]

Minimal connection: $\upsilon \cdot \kappa = \mu \cdot c$ /for some $c \in R$/

(0) <u>Homogeneous linear equations</u>:

$$\underline{A} \cdot \underline{x} = \underline{0}$$

(0) **Homogeneous linear equations**:

$$\underline{A}\cdot\underline{x} = \underline{0}$$

Find all **minimal** solutions

Acta Mathematica Academiae Scientiarum Hungaricae
Tomus 18 (1—2), 1967, pp. 19—23.

ON A CLASS OF SOLUTIONS OF ALGEBRAIC HOMOGENEOUS LINEAR EQUATIONS

By

Á. PETHŐ (Budapest)

Main Definition:

$S = \{\underline{s}_1 , \underline{s}_2 ,\ldots , \underline{s}_k \} \subset R^n$ *is an* **algebraic simplex**
iff S is minimal dependent. □
iff
S *is dependent and* $S \backslash \{\underline{s}_i\}$ *is independent* *for all* $i \leq k$. □

i.e.

$$\alpha_1 \cdot \underline{s}_1 + \alpha_2 \cdot \underline{s}_2 + \ldots + \alpha_k \cdot \underline{s}_k = \underline{0}$$

and **none** of them can be omitted : $\alpha_i \neq 0$ *for all* $i \leq k$. □

(*minimal* reactions, mechanisms, etc.)

Reminder: $S=\{\underline{s}_1, \underline{s}_2, \ldots, \underline{s}_k\} \subset R^n$ *is an algebraic* **simplex** *iff* S *is dependent and* $S \backslash \{\underline{s}_i\}$ *is independent for all* $i \leq k$. □

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TASK 1:

Algorithm for generating all simplexes $S \subset H$ in a given $H \subset R^n$.

(*all* reactions, mechanisms, etc.)

\+ Applications

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+ Applications

Result: polynomial algorithm

√ **[1991]** Hung.J.Ind.Chem. 289-292.

√ **[2000]** J.Math.Chem.1-34.

E.g.

The species:

- 1st speci: H_2
- 2nd speci: O_2
- 3st speci: HO
- 4th speci: HO_2
- 5th speci: H_2O
- 6th speci: H_2O_2

=>

1. $+ \frac{1}{2}H_2 + \frac{1}{2}O_2 - 1HO = 0$
2. $+ \frac{1}{2}H_2 + 1O_2 - 1HO_2 = 0$
3. $+ 1H_2 + \frac{1}{2}O_2 - 1H_2O = 0$
4. $+ 1H_2 + 1O_2 - 1H_2O_2 = 0$
5. $- \frac{1}{2}H_2 + 2HO_2 - 1HO_2 = 0$
6. $+ \frac{1}{2}H_2 + 1HO - 1H_2O = 0$
7. $+ \frac{3}{4}H_2 + \frac{1}{2}HO_2 - 2H_2O = 0$
8. $+ \frac{1}{2}H_2 + 1HO_2 - 1H_2O_2 = 0$
9. $- 1H_2 + 2H_2O - 1H_2O_2 = 0$
10. $+ \frac{1}{2}O_2 + 1HO - 1HO_2 = 0$
11. $+ \frac{1}{2}O_2 + 2HO - 1H_2O = 0$
12. $+ \frac{3}{2}O_2 + 2HO_2 - 1H_2O = 0$
13. $- 1O_2 + 2HO_2 - 1H_2O_2 = 0$
14. $+ \frac{1}{2}O_2 + 1H_2O - 1H_2O = 0$
15. $+ 3OH - 1HO_2 - 1H_2O = 0$
16. $+ 2OH - 1H_2O_2 = 0$
17. $+ \frac{2}{3}OH_2 + \frac{2}{3}H_2O - 1H_2O_2 = 0$

Reminder: $S=\{\underline{s}_1, \underline{s}_2, \ldots, \underline{s}_k\} \subset R^n$ *is an algebraic* **simplex** *iff* S *is dependent and* $S \setminus \{\underline{s}_i\}$ *is independent for all* $i \leq k$. □

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(*minimal* reactions, mechanisms, etc.)

Task 2:

Question: For given $H \subset R^n$ *how many* simplexes $S \subset H$ could be in H if $|H| = m$ is given and H spans R^n ?

(*how many* reactions, mechanisms, etc.)

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(*minimal* reactions, mechanisms, etc.)

Task 2:

Question: For given $H\subset R^n$ *how many* simplexes $S\subset H$ could be in H if $|H|=m$ is given and H spans R^n ?

(*how many* reactions, mechanisms, etc.)

Notation:

simp(H) := the *number* of simplexes $S\subset H$. □

Assuming: $|H|=m$, H spans R^n

Theorem 1 [1995] (Laflamme-Szalkai)

$$simp(H) \leq \binom{m}{n+1} \quad = O(m^{n+1})$$

and simp(H) *is <u>maximal</u>* ***iff*** *every* n *-element subset of* H *is independent.* □

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Note:

Sperner's theorem is not enough: what is the structure of *H* ?

$|H| = m$,   H spans R^n

Theorem 2 [1995] (Laflamme-Szalkai)

$$O(m^2) = \qquad n \cdot \binom{m/n}{2} \le simp(H)$$

and simp(H) *is* *minimal* ***iff*** m/n *elements of* H *are* ***parallel*** *to* $\underline{b}_i$ *where* $\{\underline{b}_1,\ldots,\underline{b}_n\}$ *is any base of* . □

(parallel = isomers, multiple doses,…)

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(parallel = isomers, multiple doses,…)

Open Question:

if no parallel elements are in H ?

<u>General Conjecture</u> (1998) (Laflamme, Meng, Szalkai)

no parallel => the minimal configurations in R^n are:

? 1) *If* n *is even* => H *contains* n *linearly independent vectors* $\{\underline{u}_i : i = 1,\ldots,n\}$ *and the remaining of* H *is divided as evenly as possible between the planes* $[\underline{u}_i , \underline{u}_{i+1}]$ *for* $i = 1, 3, \ldots, n - 1$. □

? 2) *If* n *is odd* => H *again contains* n *linearly independent vectors* $\{\underline{u}_i : i = 1,\ldots,n\}$, *one extra vector in the plane* $[\underline{u}_{n-1} ,\underline{u}_n]$ *and finally the remaining vectors are divided as evenly as possible between the planes* $[\underline{u}_i , \underline{u}_{i+1}]$ *for* $i = 1, 3, \ldots, n - 2$ *with lower indices having precedence.* □

LATER !

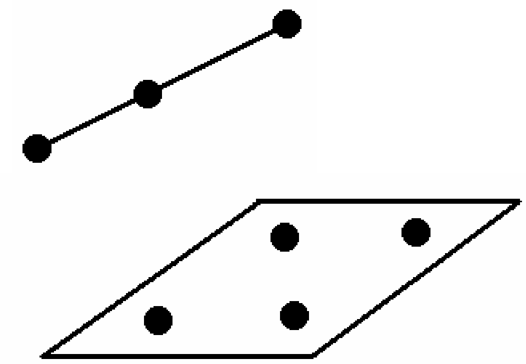
Reducing the dimension (n=3):

R^3

R^2

vectors => points, 2D-planes => lines

So, after the reduction we get:



<u>Definition:</u> **(affine) simplexes** in R^2 are

i) 3 colinear points,

ii) 4 general points: no three colinear,

□

Elementary question in R^2 :

What is the minimal number of (total) simplexes if the number of points (spanning R^2) is m ?

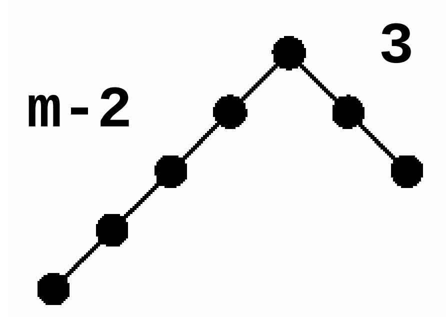
$|H|=m$, H spans R^n , no parallel elements

n=3

Theorem 3 [1998] (Laflamme-Szalkai)
For $H \subset R^3$

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

and for $m \geq 8$: simp(H) *is* *minimal* ***iff***

H = 

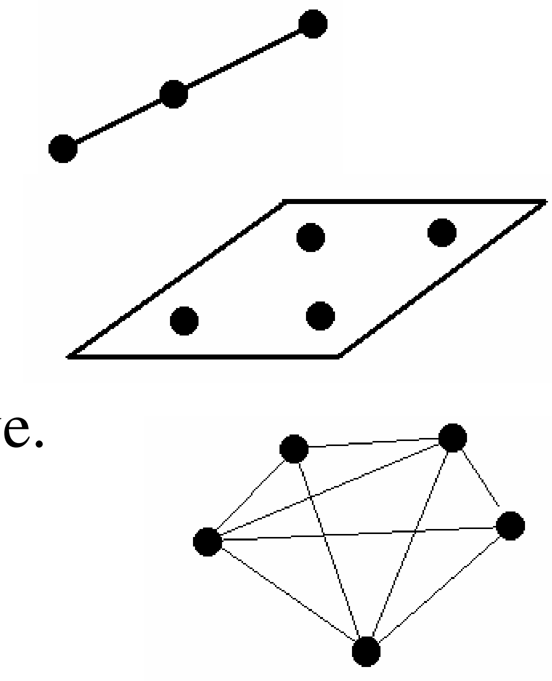
□

(vectors = points, planes = lines)

Reducing the dimension (n=4):

vectors => points, 2D-planes => lines, h.-planes **=> 2D-planes**

So, after the reduction we get:



<u>Definition:</u> **(affine) simplexes** in R^3 are

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ii) 4 coplanar, no three colinear,

iii) 5 general points: no three or four as above.

□

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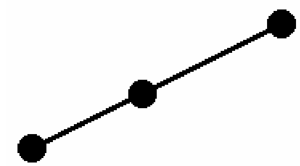

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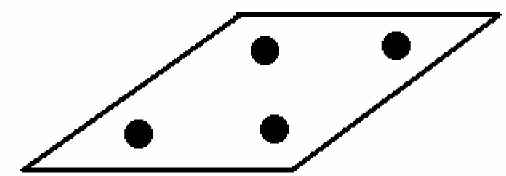

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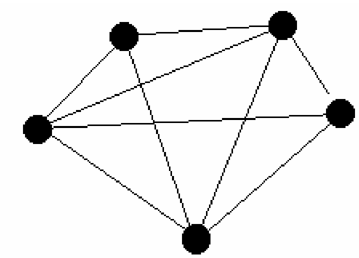
□



Still elementary question in R^3 :

What is the minimal number of (total) simplexes if the number of points (spanning R^3) is m ?

|H|=m , H spans R^n , no parallel elements

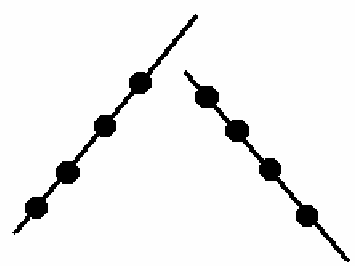
n=4

Theorem 4 [2010] (Balázs Szalkai - I.Szalkai)

For $H \subset R^4$

$$simp(\mathcal{H}) \geq \binom{\lfloor m/2 \rfloor}{3} + \binom{\lceil m/2 \rceil}{3}$$

and for m$\geq$24 simp(H) *is minimal* ***iff*** *H is placed into two (skew) detour line*



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General Conjecture (1998) (Laflamme, Meng, Szalkai)

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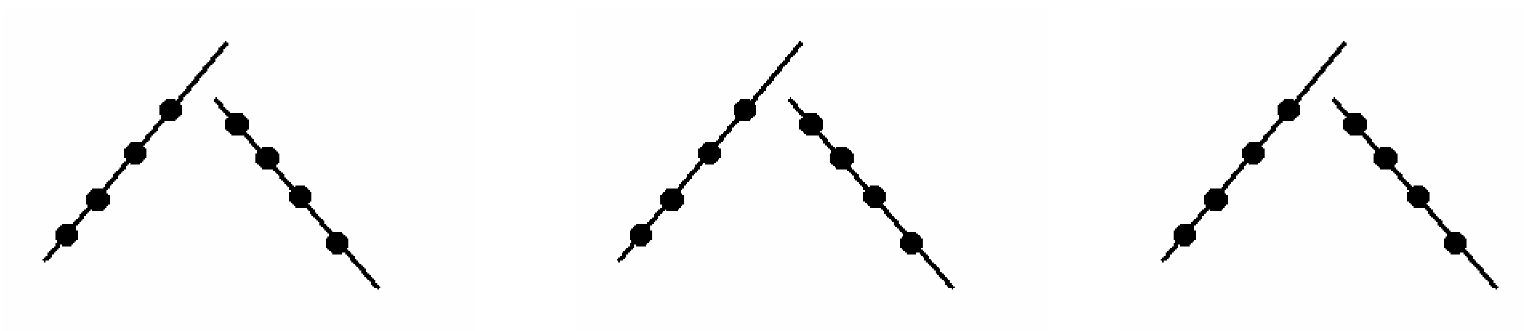

$[\underline{u}_1, \underline{u}_2]$ $[\underline{u}_3, \underline{u}_4]$ . . . $[\underline{u}_i, \underline{u}_{i+1}]$ . . . $[\underline{u}_{n-1}, \underline{u}_n]$

General Conjecture **(1998)** (Laflamme, Meng, Szalkai)
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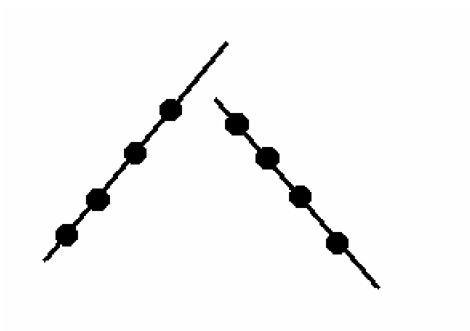
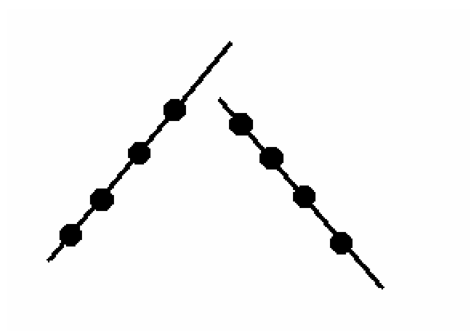
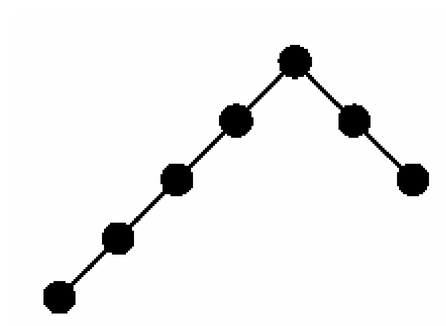

$[\underline{u}_1, \underline{u}_2]$ $[\underline{u}_3, \underline{u}_4]$ . . . $[\underline{u}_i, \underline{u}_{i+1}]$ . . . $[\underline{u}_{n-2}, \underline{u}_{n-1}]$, $[\underline{u}_{n-1}, \underline{u}_n]$

Matroids (hypergraphs) :

What is the minimal and maximal number of cycles and bases in a matroid of size **m** *and given rank* **n** *?*

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√ **[2006]** (Laflamme, Dósa, Szalkai) :

Theorem 5 *If* $m > n+1$ *then only the uniform matroid* $U_{m,n}$ *contains the maximum number of circuits:* $\binom{m}{n+1}$

If $m = n+1$ *then all matroids of size* m *and of rank* n *contain exactly* 1 *circuit.* □

Theorem 6 *If* $m > n$ *then only the uniform matroid* $U_{m,n}$ *contains the maximum number of bases:* $\binom{m}{n}$

□

Matroids (hypergraphs) :
*What is the **minimal** and maximal number of cycles and bases in a matroid of size* m *and given rank* n *?*

√ **[2006]** (Laflamme, Dósa, Szalkai) :

Theorem 7 *For each* m *and* n *there is a unique matroid* M_o *of size* m *and of rank* n *containing the minimum number of bases, namely* **1** *when we allow loops in the matroid.* □

Theorem 8 *Any matroid* M *of size* m *and of rank* n *contains the minimum number* **m-n** *circuits if and only if the circuits of the matroid are pairwise disjoint.* □

Many thanks to

You