http://math.uni-pannon.hu/~szalkai/Malta.html

Reactions, mechanisms and simplexes

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I.
Simplexes

(definitions)

(1) <u>Chemical reactions</u> :

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

<=> Linear combination of vectors

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H:      |2|       |0|     |4|     |0|     |0|
C:   2*|0| + 2*|1| - |1| - |1| = |0|
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```

No kinetics, chemics, graphs (at the end), other approaches: **/ janostothmeister@gmail.com /**

Tóth,J., Érdi,P.: *Mathematical Models of Chemical Reactions. Theory and Applications of Deterministic and Stochastic Models*, Manchester Univ. Press and Princeton Univ.Press, 1989.

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Tóth,J., Nagy,A., Papp,D.: *Reaction Kinetics: Exercises, Programs and Theorems: Mathematica for Deterministic and Stochastic Kinetics*, Springer, New York, NY, 2018.

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$$R^{C,O,H,e^-,\ldots}$$

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Idea: work in double dimension. Imagine for all species (X,Y, ...) two variants "*in*" and "*out*" and use the vectors:

$\underline{v}' + \underline{x}$

$$\underline{u}' = [-1,-1,0,...,2,0,0,...]^T \;,\quad \underline{v}' : [0,-1,0,...,1,0,0,...]^T \;,$$

and introduce the reactions "*in* ← *out*" as:

$$\underline{x} = [1,0,0,\ ...,\ -1,0,0,...]^T \;,\quad \underline{y} = [0,1,0,\ ...,0,-1,0,...]^T \;,$$

then clearly **$\underline{u} \equiv \underline{u}' + 2\underline{x}$** and **$\underline{v} \equiv \underline{v}' + \underline{x}$** ,

and modify the original "*start*" and "*goal*" reactions corres-ponding this idea.

. . . there are several more minor observations and tricks . . .

(2) Mechanisms :

1: $C + O = CO$ $\underline{x}_1 = [1,1,-1,0]$

2: $C + 2O = CO_2$ $\underline{x}_2 = [1,2,0,-1]$

(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

$$2*\underline{x}_1 - \underline{x}_2 - \underline{x}_4 = \underline{0}$$

Minimal: none of them can be omitted.
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in general:

$$\underline{Y} = \alpha_1\underline{X}_1+\alpha_2\underline{X}_2+...\alpha_n\underline{X}_n \qquad (M)$$

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$\underline{Y} := \mathbf{R}\,(M)$ = the final reaction, determined by the mechanism *(M)*

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

tube diameter	=	$d\ (\ell)$	=	[1, 0, 0, 0, 0, 0]
linear velocity	=	$v\ (s/t)$	=	[0, 1,-1, 0, 0, 0]
fluid density	=	$\rho\ (m/\ell^3)$	=	[-3, 0, 0, 1, 0, 0]
viscosity	=	$\nu\ (m/\ell t)$	=	[-1, 0,-1, 1, 0, 0]
heat capacity	=	$\kappa\ (A/t^2T)$	=	[0, 0,-2, 0, 1,-1]
heat transfer coeff.	=	$\lambda\ (m/t^3T)$	=	[0, 0,-3, 1, 0,-1]
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<=> linear combination of the exponents

$$R^{\text{exponents}}$$

(4) In General : **Main Definition:**

$S = \{\underline{s}_1, \underline{s}_2, \ldots, \underline{s}_k\} \subset R^n$ *is an (linear)* **algebraic simplex**

iff S is minimal dependent. □

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(*minimal* reactions, mechanisms, etc.)

II. System of equations

(0) Homogeneous linear equations:

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

Find the **structure** of *minimal* solutions

Question: Assuming $\mathbf{A \cdot X = 0}$, what information could be extracted from the linear /in/dependency of the *rows* and *columns* of $\mathbf{A}$ and of $\mathbf{X}$ and of $rank(\mathbf{A})$?

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columns of **A** are the "contents" of the species,

columns of **X** are the reactions,

generating/independent columns of X denote generating / independent reactions.

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rows, rank(A), rank(X) = ?

Observations (reducing the dimension)

a) *If a* column *of* A (*a species/reaction*) *is linearly* independent *fom the others, then it can be* omitted,
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c) *If a* column *of* A (*a reaction*) *contains* <u>exactly two</u> *nonzero coordinates, then this column can be* <u>omitted</u>, *since in this reaction the two species are* equivalent.

Perhaps they are important in chemistry.

NOT the Gauss elminination method.

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)

On solving algebraic homogeneous linear equations by Cramer's rule, solutions can automatically be obtained in which the number of zero elements is maximal in a sense [2]—[3]. In the present communication, these so-called „simple" solutions are defined more simply, in a combinatorial manner, and their properties are formulated more generally. The necessity of introducing simple solutions emerged originally in connection with a chemical problem [2].

$$\begin{bmatrix} a_{1,1} & a_{1,2} & a_{1,3} & \dots & a_{1,k} & \dots & a_{1,\ell} & \dots & a_{1,m-1} & a_{1,m} \\ a_{2,1} & a_{2,2} & a_{2,3} & \dots & a_{2,k} & \dots & a_{2,\ell} & \dots & a_{2,m-1} & a_{2,m} \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ a_{n,1} & a_{n,2} & a_{n,3} & \dots & a_{n,k} & \dots & a_{n,\ell} & \dots & a_{n,m-1} & a_{n,m} \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \\ \dots \\ x_m \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\underline{x} = \begin{bmatrix} 0 & x_2 & 0 & \dots & x_k & \dots & 0 & \dots & x_{m-1} & 0 \end{bmatrix}$$

$$\{i \leq m : x_i \neq 0\} := supp\,(\underline{x})$$

$\underline{\mathbf{x}}$ is *minimal* if for **no** $\underline{\mathbf{y}}$ we have $supp(\underline{\mathbf{y}}) \subset supp(\underline{\mathbf{x}})$

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$supp(\underline{\mathbf{x}}) = \{\underline{\mathbf{a}}_{i1}, \underline{\mathbf{a}}_{i2}, \dots, \underline{\mathbf{a}}_{ik} : x_{ij} \neq 0\}$

Notation $M_{A,\underline{b}}$ *and* $M_{A,\underline{0}}$ *denote the sets of solutions of* $A\cdot\underline{x} = \underline{b}$ *and* $A\cdot\underline{x} = \underline{0}$ □

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Condition

o) $M_{A,\underline{0}} \neq \{\underline{0}\}$ *and* $|M_{A,\underline{b}}| > 1$,

i) *A has no parallel columns, especially*

ii) *A has no column* $\underline{0}$,

iii) *A has no column parallel to* $\underline{b}$. □

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iii) *A has no column parallel to* $\underline{b}$. $\Box$

Definition *(i)* *For any* $\underline{x} \in \mathbb{R}^m$

$$\mathbf{supp}\,(\underline{x}) := \{i \le m : x_i \neq 0\}$$

the ***support*** *of* $\underline{x}$, *especially* $\mathbf{supp}\,(\underline{0}) = \emptyset$.

(ii) *For* $M \subseteq \mathbb{R}^m$ *the vector* $\underline{z} \in M$, $\underline{z} \neq \underline{0}$ *has a* ***minimal support*** *with respect to M* ($\underline{z}$ *is* ***minimal*** *to M*)

if there is no $\underline{y} \in M$, $\underline{y} \neq \underline{0}$ *such that* $\mathrm{supp}\,(\underline{y}) \subsetneq \mathrm{supp}\,(\underline{z})$.

(iii) *For any* $M \subseteq \mathbb{R}^m$

$$M^{\min} := \{\underline{z} \in M : \underline{z} \text{ is minimal to } M\} .$$

Proposition *For any* $\underline{z} \in M^{\min}_{A,\underline{0}}$, $A \cdot \underline{z} = \underline{0}$,

the relevant set of column vectors of A

$$S_{\underline{z}} := \{\underline{a}_i : i \in supp\,(\underline{z})\} \subset \mathbb{R}^n$$

is a <u>*simplex*</u> (minimal *dependent set*) . $\square$

Connection of minimal- and base solutions:

Inhomogeneous *systems:*

A base solution $\underline{x}$ *corresponds to a base of A but some components of* $\underline{x}$ *may be* 0 .

$\underline{x}$ *is* minimal iff *it is* nondegenerate.

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Homogeneous *systems:*

each base solution refers to a base *of* A and *a further column of* A, *this is an* $r+1$ *-element dependent vectorset ,* $r = rank(A)$.

Such set need not be a simplex .

On the other hand: minimal solutions $\underline{x}$ *correspond to simplexes, they are base solutions* <=> $supp(x) = r+1$. $\square$

homogeneous systems

Theorem $M^{\min}_{A,\underline{0}} \subseteqq \mathbb{R}^m$ *generates* $M_{A,\underline{0}} \subseteqq \mathbb{R}^m$ *for any* $A \in \mathbb{R}^{n\times m}$. □

Corollary *For any* $\underline{x} \in M_{A,\underline{0}}$

$$supp\,(\underline{x}) \;\subseteqq\; \bigcup \left\{ supp\,(\underline{z}) : \underline{z} \in M^{\min}_{A,\underline{0}} \right\} \;. \quad \square$$

Remark $M^{\min}_{A,\underline{0}}$ *may contain dependent but not parallel elements.*

To reveal a base *of* $M^{\min}_{A,\underline{0}}$ *would be interesting.* □

Inhomogeneous systems

Theorem *For any* $\underline{z} \in M^{\min}_{A,\underline{b}}$, $H := supp\,(\underline{z})$

$$(A \mid_H) \cdot \underline{y} = \underline{b}$$

has the only solution $\underline{y} = \underline{z} \mid_H$. $\square$

Problem *Can **all** solutions of* $A \cdot \underline{x} = \underline{b}$ *be generated from the* minimal *solutions, i.e. from* $M^{\min}_{A,\underline{b}}$ *?*

Theorem *Each solution* $\underline{x} \in M_{A,\underline{b}}$

$$\underline{x} = \sum_{i=1}^{I} \alpha_i \underline{z}_i + \underline{y}$$

where $\underline{z}_i \in M_{A,\underline{b}}^{\min}$, $\sum_{i=1}^{I} \alpha_i = 1$, $\underline{y} \in M_{A,\underline{0}} \cup \{\underline{0}\}$,

i.e. is an affine *linear combination of the elements* $M_{A,\underline{b}}^{\min}$ plus *one solution of* $M_{A,\underline{0}}$. $\square$

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Corollary $M_{A,\underline{b}}^{\min} \cup M_{A,\underline{0}}^{\min}$ *generates* $M_{A,\underline{b}}$. □

This is a generalization of the wellknown

$$M_{A,\underline{b}} = \underline{z} + M_{A,\underline{0}} \ .$$

III.
Algorithm

(0) Homogeneous linear equations:

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

Find all **minimal** solutions

Happel-Sellers-Otarod [HOS,1990] 's **algorithm** for reaction-mechanisms uses :

- mainly *elementary matrix row-column* operations
- *eliminating equations*.

after reductions:

- determine the bases of the solutions with *heuristic* methods.

Their method is mainly theoretical, non automatic.
No further details are published.

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* $i \leq k$. □

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.

(*minimal* reactions, mechanisms, etc.)

Our 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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Result: polynomial algorithm

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

√ **[2000]** J. Math. Chem.1-34.

The algorithm

Each simplex in $\mathbb{R}^n$ has size at most $n+1$,

$|H| = m$ => H has at most

$$\sum_{i=1}^{n+1} \binom{m}{i} = \binom{m+1}{n+2} - 1 = \mathcal{O}\left(m^{n+2}\right)$$

such subsets.

The algorithm

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such subsets.

However we do not have to check these m^{n+2} subsets, since

Proposition *All subsets of independent sets are independent, too.* $\square$

Procedure Modify

szimplex[ ] := {1} ;
while not end do begin
if szimplex[ ] $= \{k, k+1, \ldots, M, c\}$ **and** $c \neq$ "d" **then END;**
if szimplex[ ] $= \{k, k+1, \ldots, M,$ "d"$\}$
then $S := \{k, k+1, \ldots, M-2, M,$ " "$\}$;
if szimplex[ ] $= \{T, t, M, c\}$ **then** $S := \{T, t+1,$ " "$\}$;
if szimplex[ ] $= \{T, t,$ "i"$\}$ **then** $S := \{T, t, t+1,$ ""$\}$;
if szimplex[ ] $= \{T, t,$ "d"$\}$ **then** $S := \{T, t+1,$ " "$\}$;
if szimplex[ ] $= \{T, t,$ "s"$\}$ **then** $S := \{T, t+1,$ " "$\}$;

end ;

Definition 13 *(PhD 2.4.D.)* ***(i)*** *A hypergraph* $\mathcal{H} = (V, \mathcal{E})$ *is* ***descending*** *if* $E, F \subseteqq V$, $E \in \mathcal{E}$ *and* $F \subset E$ *implies* $F \in \mathcal{E}$,
(ii) $\mathcal{H}$ ***is not deformed*** *if* $\{v\} \in \mathcal{E}$ *for each* $v \in V$,
(iii) *assumed (i) and (ii), the elements of* $\mathcal{E}$ *are called* ***independent,***
(iv) $S \subseteqq V$ *is a* ***simplex*** *if* $S \notin \mathcal{E}$ *but for each* $T \subsetneqq S$ *we have* $T \in \mathcal{E}$. □

Definition 13 ***(PhD 2.4.D.) (i)*** *A hypergraph $\mathcal{H} = (V, \mathcal{E})$ is* ***descending*** *if $E, F \subseteqq V$, $E \in \mathcal{E}$ and $F \subset E$ implies $F \in \mathcal{E}$,*
(ii) *$\mathcal{H}$* ***is not deformed*** *if $\{v\} \in \mathcal{E}$ for each $v \in V$,*
(iii) *assumed (i) and (ii), the elements of $\mathcal{E}$ are called* ***independent****,*
(iv) *$S \subseteqq V$ is a* ***simplex*** *if $S \notin \mathcal{E}$ but for each $T \subsetneqq S$ we have $T \in \mathcal{E}$.* □

Theorem 14 ***(PhD 2.2.T.) (i)*** *The algorithm does not miss any simplex and does not check any subset twice.*
(ii) *The running time of the algorithm is the best possible for any dataset, that is it checks the neccessary ones only.* □

Theorem 15 ***(PhD 2.3.T.)*** *For any $H \subset \mathbb{R}^n$, $|H| = m$ the algorithm checks at most m^{n+1} subsets of H , so the time elapsed is $\mathcal{O}(m^{n+1})$, the algorithm is polynomial in time.* □

Computer examples are shown in the last Section of the dissertation: for some dozens of vectors in dimension $10 - 20$ we have result in some seconds.

The time $\mathcal{O}(m^{n+1})$ can not be decreased in general, by Theorem 32 and Corollary 33.

J.Tóth, A.Nagy, D.Papp:

Reaction Kinetics: Exercises, Programs and Theorems: Mathematica *for Deterministic and Stochastic Kinetics.*

Springer, New York, NY, 2018. ISBN:9781493986415,

IV. Examples

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. $+\frac{2}{3}OH_2 + \frac{2}{3}H_2O - 1H_2O_2 = 0$

"Amundson" ([A66], [P90])

$CO, CO_2, O_2, H_2, CH_2O, CH_3OH, C_2H_5OH, (CH_3)_2CO, CH_4,$

CH_3CHO, H_2O = 11 vektor 3 -dim, 213 szimplex 0.22 mp.

$$-2CO + 2CO_2 - O_2 = 0 \ ,$$
$$3CO - CO_2 + 3H_2 - C_2H_5OH = 0 \ ,$$
$$5CO - 2CO_2 + 3H_2 - C_2H_6CO = 0 \ ,$$
$$2CO - CO_2 + 2H_2 - CH_4 = 0 \ ,$$
$$3CO - CO_2 + 2H_2 - CH_3CHO = 0 \ ,$$
$$-1CO + CO_2 + H_2 - H_2O = 0 \ , \quad \ldots$$

N (vektortér dimenziója)	3
n (a H által kifeszített altér dimenziója)	3
M (input vektorok száma: $\|H\|$)	11
$simp(H)$ (szimplexek tényleges száma)	213
$1 + \binom{M-2}{3} + \binom{M-3}{2}$ (alsó becslés)	$113 \leq$
$\binom{M}{n+1}$ (felső becslés)	≤ 330
t (futásidő $[mp]$)	$0.22\ mp$
H vizsgált részhalmazainak száma	502

"Metán" ([B99], [HS83])

szintézise szénmonoxidból és vízből, $\mathbf{S}_R$ reakciót kell előállítani $S_1 - S_{15}$ -ból (ℓ a katalizátor):

$\mathbf{S}_R$: $\mathbf{2H_2{+}2CO \rightarrow CH_4{+}CO_2}$,

$S_1 : CO\ell + \ell = C\ell + O\ell$, $S_2 : C\ell + H\ell = CH\ell + \ell$,

$S_3 : CH\ell + H\ell = CH_2\ell + \ell$, $S_4 : CH_2\ell + H\ell = CH_3\ell + \ell$,

$S_5 : CH_3\ell + H\ell = CH_4 + 2\ell$, $S_6 : OH\ell + H\ell = H_2O + 2\ell$,

$S_7 : CO_2 + \ell = CO_2\ell$, $S_8 : CO + \ell = CO\ell$,

$S_9 : H_2 + 2\ell = 2H\ell$, $S_{10} : CO_2\ell + H\ell = CHOO\ell + \ell$

$S_{11} : CHOO\ell + H\ell = CHO\ell + OH\ell$,

$S_{12} : O\ell + H\ell = OH\ell + \ell$, $S_{13} : CO\ell + O\ell = CO_2\ell + \ell$,

$S_{14} : CHOO\ell + \ell = OH\ell + CO\ell$, $S_{15} : CO\ell + H\ell = CHO\ell + \ell$

Az összes minimális mechanizmus (output):

1) $S_1 + S_2 + S_3 + S_4 + S_5 - S_7 + 2S_8 + 2S_9 - S_{10} - S_{11} + S_{12} + S_{15} = S_R$

2) $S_1 + S_2 + S_3 + S_4 + S_5 - S_7 + 2S_8 + 2S_9 - S_{10} + S_{12} - S_{14} = S_R$

3) $S_1 + S_2 + S_3 + S_4 + S_5 - S_7 + 2S_8 + 2S_9 + S_{13} = S_R$

4) $S_{10} + S_{11} - S_{12} + S_{13} - S_{15} = 0$

5) $S_{10} - S_{12} + S_{13} + S_{14} = 0$

6) $S_{11} - S_{14} - S_{15} = 0$

(Az utolsó három csak ciklus.)

	Összesen	Csak S_R -t tartalmazók
N (vektortér dimenziója)	17	17
n (a H által kifeszített altér dimenziója)	13	13
M (input vektorok száma: $\|H\|$)	16	16
$simp(H)$ (szimplexek száma)	6	3
$b \cdot \binom{a+1}{2} + (n-b) \cdot \binom{a}{2}$ (alsó becslés)	$4 \leq$	$1 \leq$
$\binom{M}{n+1}$ (felső becslés)	≤ 120	≤ 105
t (futásidő $[mp]$)	78.60 s	43.28 s
H vizsgált részhalmazainak száma	63 429	31 697

"Metán"

7.3. Táblázat

V.
Number of simplexes

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* $i \leq k$. □

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.

(*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.)

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

i.e. $\alpha_1 \cdot \underline{s}_1 + \alpha_2 \cdot \underline{s}_2 + \dots + \alpha_k \cdot \underline{s}_k = \underline{0}$ and none of them can be omitted.

(*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)

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

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

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

Theorem 1 [1995] (Laflamme-Szalkai)

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

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

Notes:

- Sperner's theorem is not enough: what is the structure of *H* ?
- Vandermonde determinant: $x_i = [1,\lambda_i,\dots,\lambda_i^{n-1}]^T$ ($i=1,\dots,m$)
- species are built from *n* particles and any *n* species are independent (and any *n*+1 are dependent) .

Proof. $|\mathcal{H}| = m$, $[\mathcal{H}] = \mathbb{R}^n$, $\mathcal{V} \subseteq \mathcal{H}$ is a base.

If $u \in \mathcal{H} \backslash \mathcal{V}$ and $u \in \mathcal{D} \subseteq \mathcal{H}$ dependent, $|\mathcal{D}| \leq n$ then

choose $u' \in \mathbb{R}^n$ s.t. $u' \notin [h_1, ..., h_{n-1}]$ for any $\{h_1, ..., h_{n-1}\} \subseteq \mathcal{H}$ and let

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

Proof. $|\mathcal{H}| = m$, $[\mathcal{H}] = \mathbb{R}^n$, $\mathcal{V} \subseteq \mathcal{H}$ is a base.

If $u \in \mathcal{H} \backslash \mathcal{V}$ and $u \in \mathcal{D} \subseteq \mathcal{H}$ dependent, $|\mathcal{D}| \leq n$ then choose $u' \in \mathbb{R}^n$ s.t. $u' \notin [h_1, ..., h_{n-1}]$ for any $\{h_1, ..., h_{n-1}\} \subseteq \mathcal{H}$ and let

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

Then for any simplex $\mathcal{S} = \{u_1, u_2, ..., u_k\} \subseteq \mathcal{H}$ $(k \leq n+1)$:

- if $u \notin \mathcal{S}$ then $\mathcal{S}$ is still a simplex of $\mathcal{H}'$,
- if $u \in \mathcal{S}$, say $u = u_i$, then $\mathcal{S} \backslash \{u_i\}$ is independent,

so $\mathcal{S} \backslash \{u_i\} \cup \mathcal{V}'$ is independent, too, and spans $\mathcal{R}^n$ for some $\mathcal{V}' \subseteq \mathcal{V}$.

Now

$$\mathcal{S}' := \mathcal{S} \backslash \{u_i\} \cup \mathcal{V}' \cup \{u'\}$$

is a new simplex of $\mathcal{H}'$.

The map $\mathcal{S} \to \mathcal{S}'$ is one-to-one, so $simp(\mathcal{H}') \geq simp(\mathcal{H})$.

No other configuration has so many simplexes:

$\mathcal{S} \subseteq \mathcal{H}$ be fixed, $|\mathcal{S}| = \ell$,

the above construction repeatedly $m - \ell$ many times $\Longrightarrow$

no $u \in \mathcal{H}' \backslash \mathcal{S}$ belongs to any subspace generated my $n-1$ elements of $\mathcal{H} \backslash \{u\}$.

No other configuration has so many simplexes:

$\mathcal{S} \subseteq \mathcal{H}$ be fixed, $|\mathcal{S}| = \ell$,

the above construction repeatedly $m - \ell$ many times $\Longrightarrow$

no $u \in \mathcal{H}' \setminus \mathcal{S}$ belongs to any subspace generated my $n-1$ elements of $\mathcal{H} \setminus \{u\}$.

Now simplexes in $\mathcal{H}$: $\mathcal{S}$ itself,

and only $n+1$ element simplexes which contain at most $\ell - 1$ elements of $\mathcal{S}$

$$simp(\mathcal{H}) \leq 1 + \sum_{i=0}^{\ell-1} \binom{\ell}{i} \cdot \binom{m-\ell}{n+1-i} = 1 + \binom{m}{n+1} + \binom{m-\ell}{n+1-\ell} < \binom{m}{n+1}$$

whenever $n + 2 \leq m$. $(n + 1 \geq m$ easy). ■

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

Theorem 2 [1995] (Laflamme-Szalkai)

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

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,…)

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

Theorem 2 [1995] (Laflamme-Szalkai)

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

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* . □

Proof: similar packing vectors to parallel sets to a base to reduce *simp*(H) .

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

Theorem 2 [1995] (Laflamme-Szalkai)

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

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* . □

More precisely:

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

where

$$m = an + b \quad , \quad 0 \leq b < n \ , \quad a \geq 1 \ .$$

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

Theorem 2 [1995] (Laflamme-Szalkai)

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

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

Open Question:

if <u>no parallel</u> elements are in H ?

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

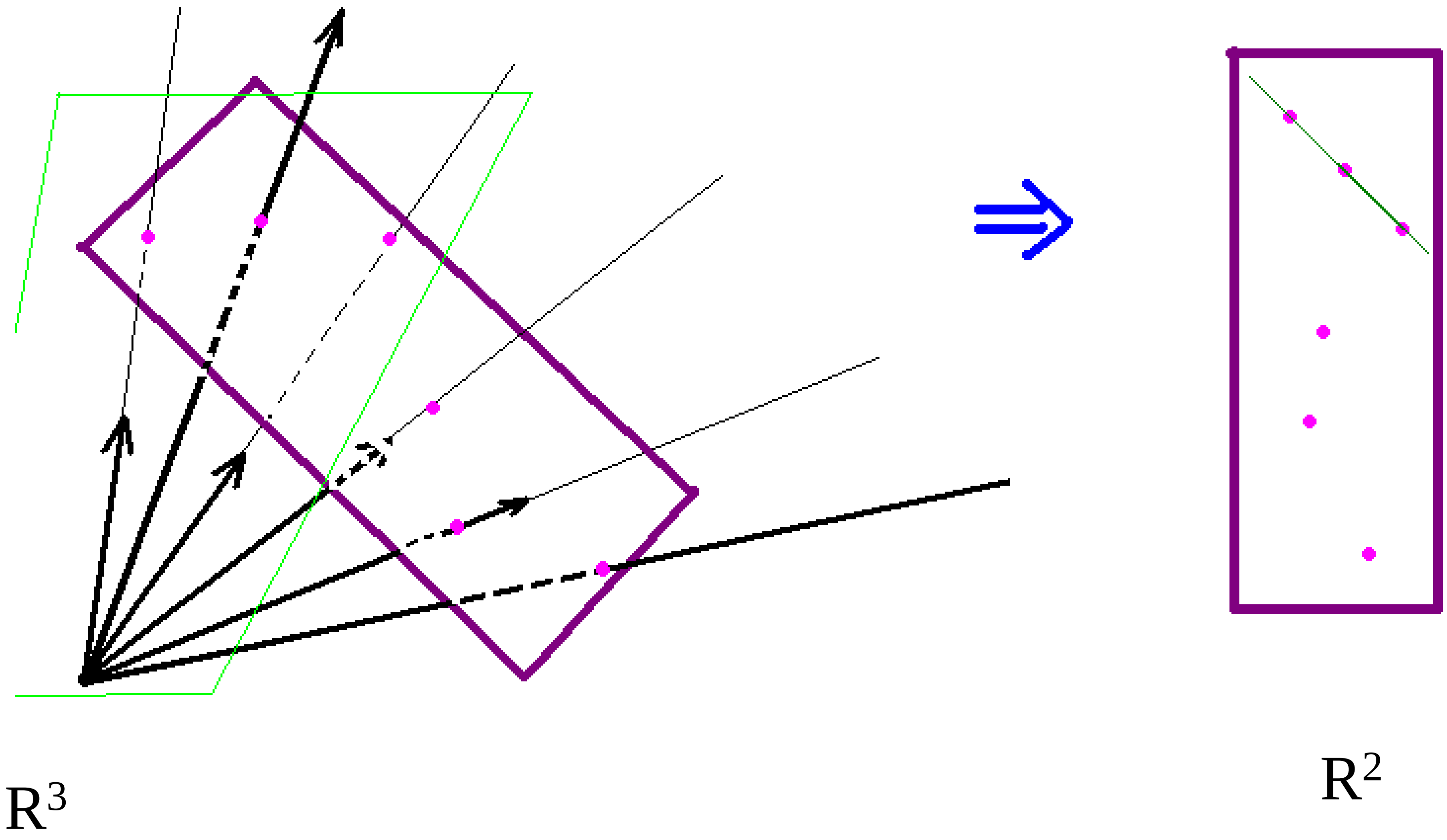
no parallel => the minimal configurations in R^n are:

? 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.* □

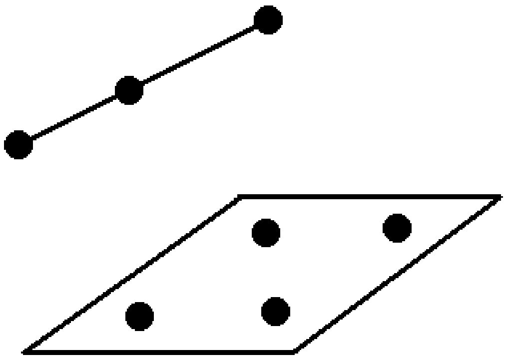
LATER !

Reducing the dimension (n=3):



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

So, after the reduction we get:



<u>Definition:</u> **(affine) simplexes** in $\mathbf{R}^2$ 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

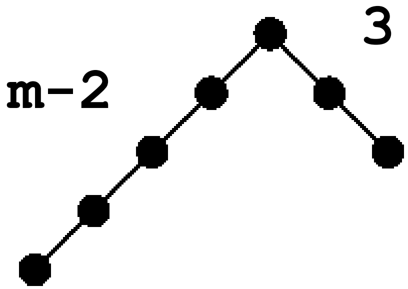
Theorem 3 [1998] (Laflamme-Szalkai)

For $H \subset R^3$

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

and for m≥8 :   simp(H) *is* *minimal*   ***iff***

H =



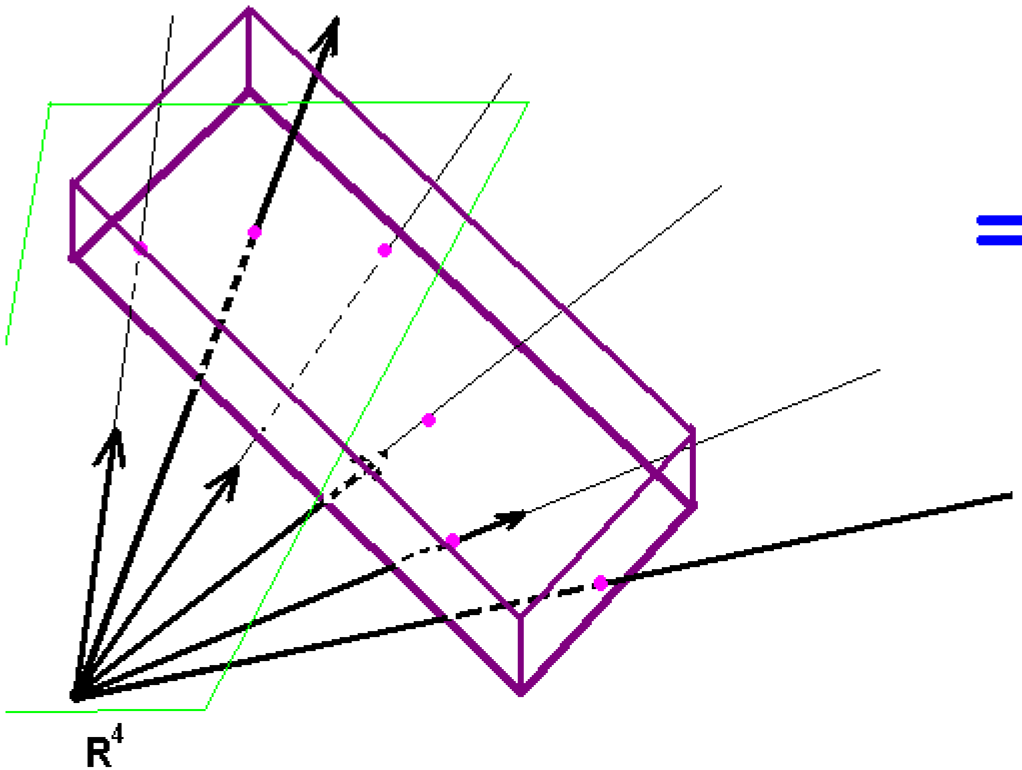
□

(vectors = points,   planes = lines)

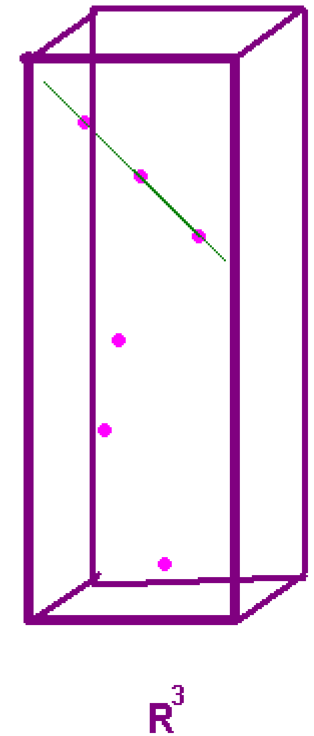
Theorem 3 [1998] (Laflamme-Szalkai)

Proof: packing points to lines to reduce *simp*(H),
many subcases, 14 pp long.

Reducing the dimension (n=4):

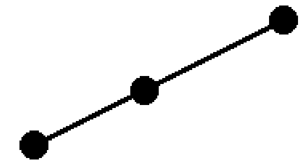


⇒

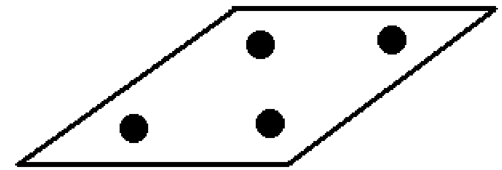


vectors => points, 2D-planes => lines, h.-planes **=> 2D-planes**

So, after the reduction we get:



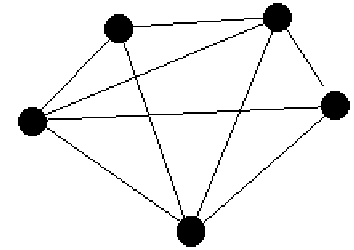
<u>Definition:</u> **(affine) simplexes** in $\mathbf{R}^3$ are



i) 3 colinear points,

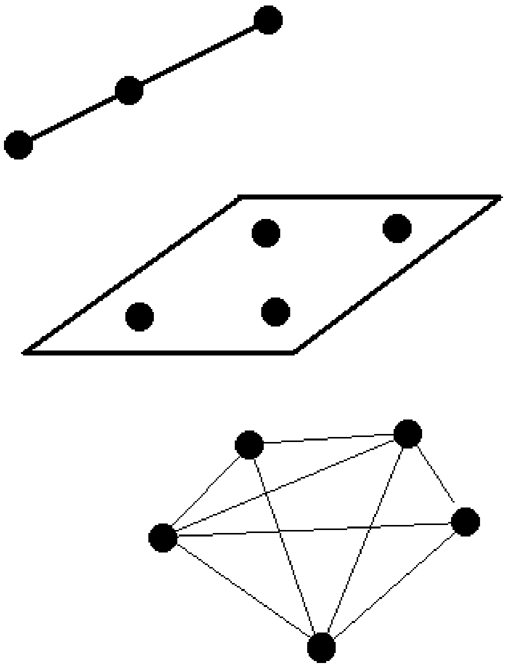
ii) 4 coplanar, no three colinear,

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



□

So, after the reduction we get:



<u>**Definition:**</u> **(affine) simplexes** in $\mathbf{R}^3$ are

i) 3 colinear points,

ii) 4 coplanar, no three colinear,

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

□

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

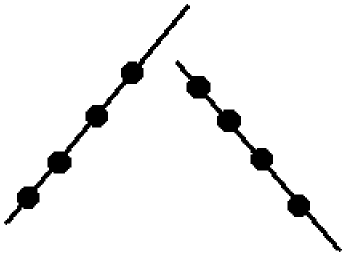
n=4

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

For $H \subset \mathbf{R}^4$

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

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



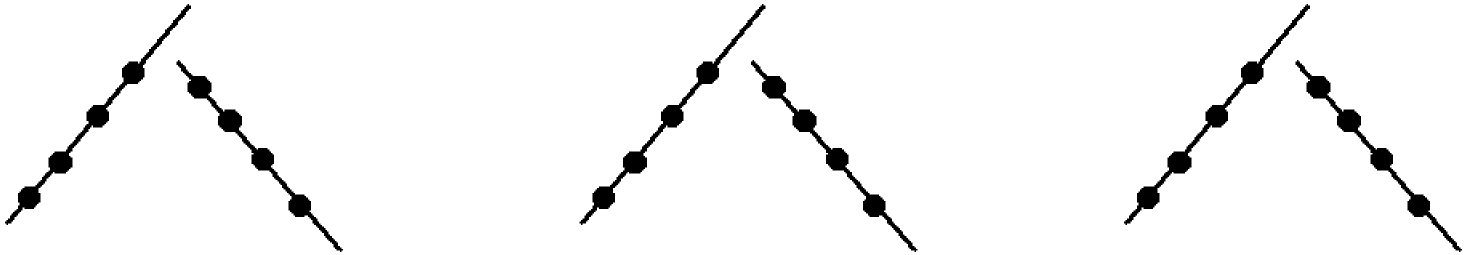
□

Theorem 4 [2010] (Laflamme-Szalkai)

Proof: packing points to planes to reduce *simp*(H),
using the infinite sides of a tetrahedron
many subcases, 10 pp long.

General Conjecture **(1998)** (Laflamme, Meng, Szalkai)
no parallel => the only minimal configurations in R^n are:

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

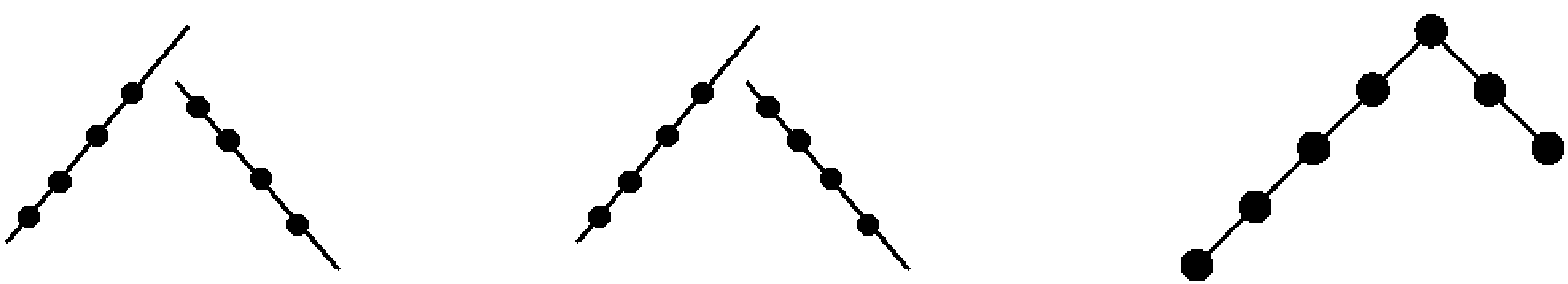


$[\underline{u}_1, \underline{u}_2]$ $[\underline{u}_3, \underline{u}_4]$ . . . $[\underline{u}_i, \underline{u}_{i+1}]$ . . . $[\underline{u}_{n-1}, \underline{u}_n]$

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

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

? 2) *If* n *is odd* => H *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.* □



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

VI.
Matroids

Matroids (hypergraphs) :

What is the <u>*minimal*</u> *and* <u>*maximal*</u> *number of* <u>*cycles*</u> *and* <u>*bases*</u> *in a matroid of size* **m** *and given rank* **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 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.* □

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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□

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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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.* □

THM: *For each m and n each matroid* M *contains the* *minimum* *number of* *bases* ***iff*** *it has a base* $\{a_1, a_2, \ldots, a_n\}$ *such that all other elements in M are* ***parallel*** *to* a_1 .

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PROBLEM *Characterize the matroids with the minimum number of circuits and bases, when neither parallel elements nor loops are allowed.*

Conjecture [Oxley, 1997] *For matroids with* $\boldsymbol{k} \leq$ **girth(M)** *the uniform matroid* $U_{m-3,k}$ *has minimal number of circuits, namely*

$$1 + 3 \cdot \binom{m-3}{k-1} + 3 \cdot \binom{m-3}{k-2} + \binom{m-3}{k-3}$$

THM. [2015] (Alahmadi,Aldred,Cruz,Ok,Solé,Thomassen) :
Any loopless matroid M *of size* μ *and rank* ν *without parallel elements has* <u>*at least*</u> μ <u>*cocircuits*</u> .

VII.
Codes, Families, …

DEF: *For* $n,k \in \mathrm{N}$ *and* $\mathrm{C} \in \boldsymbol{C}[n,k]$ ***linear code*** (*length n dimension k*)

$\mathrm{M(C)}$:= *number of <u>minimal</u> codewords in* C

and $\mathrm{M}(n,k)$:= $\underline{\max}$ $\{ \mathrm{M(C)} \mid \mathrm{C} \in \boldsymbol{C}[n,k] \}$.

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circles of matroids => $\mathrm{M}(n,k) \leq \binom{n}{k-1}$

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THM. [2015] (Alahmadi,Aldred,Cruz,Ok,Solé,Thomassen) :

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M(C) := *number of minimal codewords in* C

and M(*n,k*) := max { M(C) | C∈***C***[*n,k*] } .

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THM. [2015] (Alahmadi,Aldred,Cruz,Ok,Solé,Thomassen) :

C *has distances* ≥ 2, *circles of matroids* =>

$$b\binom{a+1}{2} + (n-k-b)\binom{a}{2} \le M(n,k) \qquad / \; n = a \cdot (n-k)+b \; /$$

Corollary [2015] (Alahmadi,Aldred,Cruz,Ok,Solé,Thomassen, Kashyap) :

For any [n,k] ***code*** C *of dual distance at least* 3 : $M(C) \geq n$

G is a connected graph (allowing multiple edges but no loops),
p vertices, **q** edges.

QUESTION [1981] (Entringer and Slater):
How many cycles $\#C_G$ *a graph with* p *vertices and* q *edges can have*?

Trivial: $\#C_G < 2^{q-p+1}$

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Cycle code **C(G)** has *length* **n**=q, *dimension* **k** = q−p+1.

Note: The minimal codewords of C(G) are exactly the incidence vectors of cycles, that is, circuits in the cycle matroid in G.

THM. [2013] (Aldred,Alahmadi,Cruz,Solé,Thomassen) :
If $q>2p+O(\log(p))$ *then* $\#C_G < 2^{q-p}$.

THM. [2015] (Alahmadi,Aldred,Cruz,Ok,Solé,Thomassen) :
matroids => In any 2-*edge-connected* ***graph*** *with p vertices and q edges the number of cycles is* (the bound is tight) /$q=a(p-1)+b$/

$$b\binom{a+1}{2}+(p-1-b)\binom{a}{2} \leq \#C_G$$

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THM. [2015] (Alahmadi,Aldred,Cruz,Ok,Solé,Thomassen) :
Any 2-connected graph with q edges and p vertices contains at least

$$\binom{q-p+2}{2} \leq \#C_G$$

DEF: Let $m, d \in \mathbb{N}$, $\mathcal{X}_m := \{1, ..., m\}$ and

$\mathcal{P}(\mathcal{X}_m) := \{p : \mathcal{X}_m \to \mathbb{R} \mid p \text{ is a probability measure on } \mathcal{X}_m\}$.

Then, for any fixed $q \in \mathcal{P}(\mathcal{X}_m)$ and $A = [\underline{a}_1, ..., \underline{a}_m] \in \mathbb{R}^{d \times m}$ let

$$\mathcal{E}_{q,A} := \left\{ s \in \mathcal{P}(\mathcal{X}_m) \;\middle|\; s(i) = \frac{q(i) \cdot \exp\left(\underline{\theta}^T \underline{a}_i\right)}{\sum_{j=1}^{m} q(j) \cdot \exp\left(\underline{\theta}^T \underline{a}_j\right)} \text{ for } i \leq m,\; \underline{\theta} \in \mathbb{R}^d \right\}$$

an "**exponential family**". □

THM: [Rauh,Kahle,Ay,2009] Any $p \in \mathcal{P}(\mathcal{X}_m)$ is in the <u>closure</u> of $\mathcal{E}_{q,A}$ **iff**

$$p^{u^+} \cdot q^{u^-} = p^{u^-} \cdot q^{u^+} \text{ for all } u \in Ker(A)$$

where $p^v := \prod_{\substack{i=1 \\ 0<v(i)}}^{m} p(i)^{v(i)}$ and u^+, u^- are the + and - components of $u \in \mathbb{R}^m$.

NOTE: Using the estimates on the number of circuits of matroids, the number of equations above is at most $\binom{m}{r+2}$ where $r = \dim(\mathcal{E}_{q,A})$.

VIII. Hypergraphs

Definition *For any hypergraph* $\mathcal{H} = (V, \mathcal{E})$, $V \neq \emptyset$, $k \in \mathbb{N}$ 1'st version

(i) $\mathcal{E}_k := \{E \in \mathcal{E} \ : \ |E| = k\}$,

(ii) *any* k*-element subset of* V *is* k***-vertex,***

(iii) $S \subset V$ *is* ***in general position*** *if*

$$S \nsubseteq E \quad \text{for all } E \in \mathcal{E} \ ,$$

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(iv) S *is* k***-pyramid*** *if it is a* k*-vertex in general position,*

(v) 4*-vertices are* ***quads***, 4*-pyramids are* ***tetrahedrons,***

(vi) $S \subset V$ *is a* 4*-element* ***simplex*** *if it is a quad but not a tetrahedron:*

$$S \subseteq E \quad \text{for some } E \in \mathcal{E} \ ,$$

$\mathcal{S}_4$ *is the* set *of the* 4*-element simplexes,* 1'st version

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$\mathcal{S}_4$ *is the* set *of the* 4*-element simplexes,*

(vii) $T \subset V$ *is a* 5*-element* ***simplex*** *if it is a* 5*-vertex but no its subset is a* 4*-element simplex:*

$$F \nsubseteq T \quad \text{for all } F \in \mathcal{S}_4 \ , \quad \text{i.e.} \quad |T \cap E| \leq 3 \text{ for } E \in \mathcal{E} \ ,$$

$\mathcal{S}_5$ *is the* set *of the* 5*-element simplexes.* □

Condition

i) $\mathcal{E}_\ell = \emptyset \quad \textit{for}\ \ell \leq 3\ ,$

ii) $\textit{for any}\ E_1, E_2 \in \mathcal{E},\ E_1 \neq E_2 \qquad |E_1 \cap E_2| \leq 2\ .$ $\square$

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Problem *If* $|V| = m$, *what is the* minimal *value of*

$$s(m) := |\mathcal{S}_4| + |\mathcal{S}_5| \qquad ?$$ □

1'st version

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Theorem 65 *Under Condition and* $m \geq 58$ *we have a constant* $C_1 \leq 17$

$$\binom{m}{4} - \frac{1}{6} C_1 m^3 - \mathcal{O}\left(m^2\right) \quad \leq \quad s(m)$$ □

(Zs.Tuza, I.Szalkai, 2013)

Recall: **2'nd version**

Problem 2 *What is* ***min*** *simp* $(\mathcal{V})$ *and the* ***structure*** *of* $\mathcal{V}$ *if* $[\mathcal{V}] = \mathbb{R}^D$, $|\mathcal{V}| = m$ *and no parallel vectors in* $\mathcal{V}$ *?*

($S_\ell \subseteqq \mathcal{V}$ linear algebraic *simplexes)*

Recall: **2'nd version**

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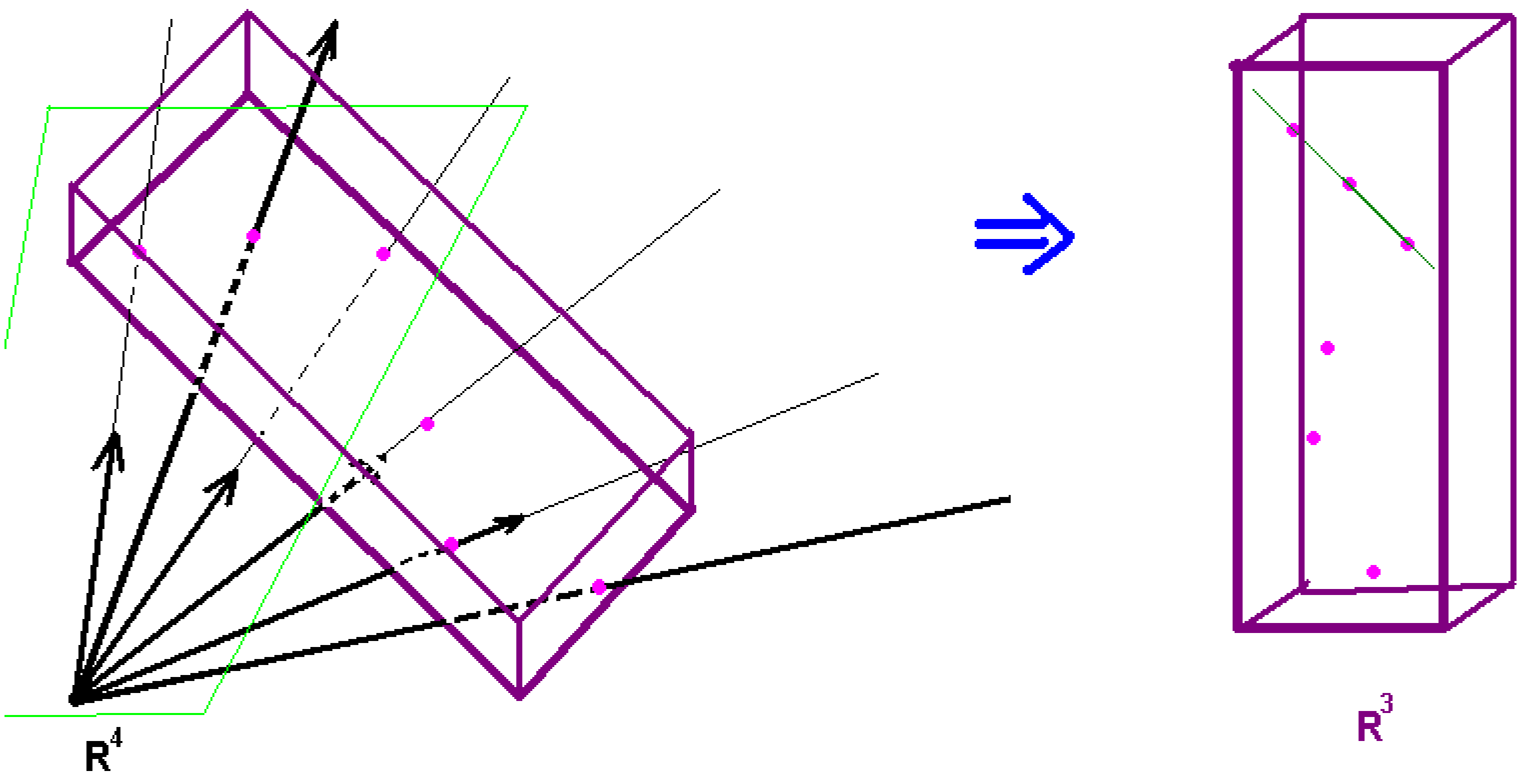
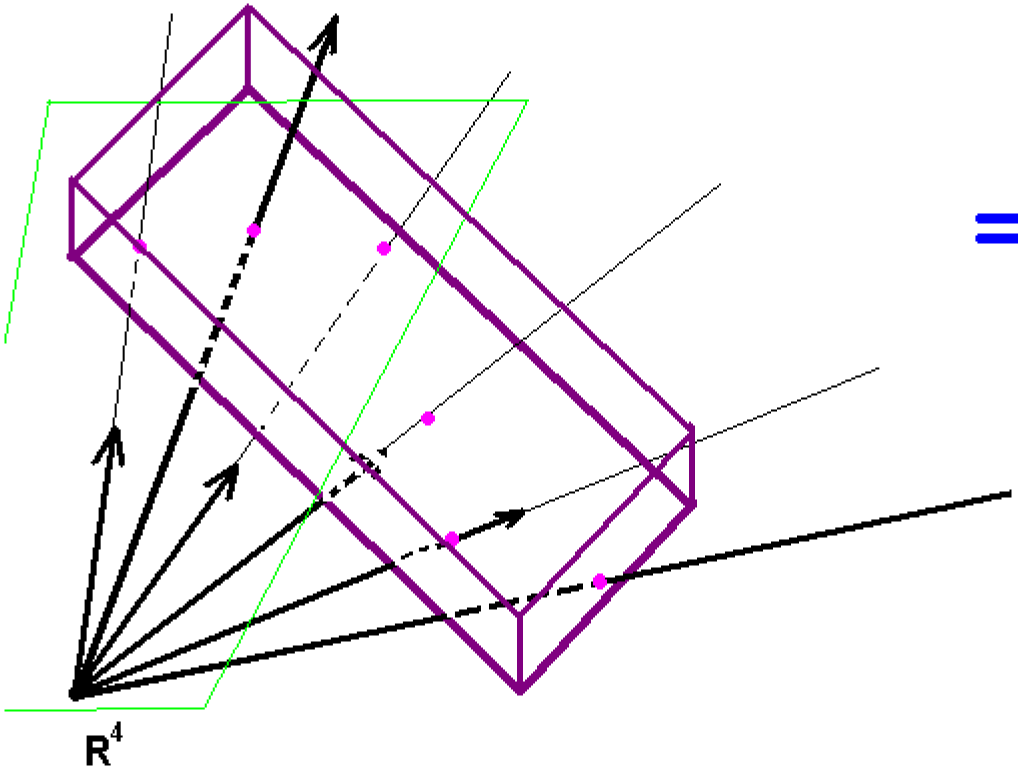
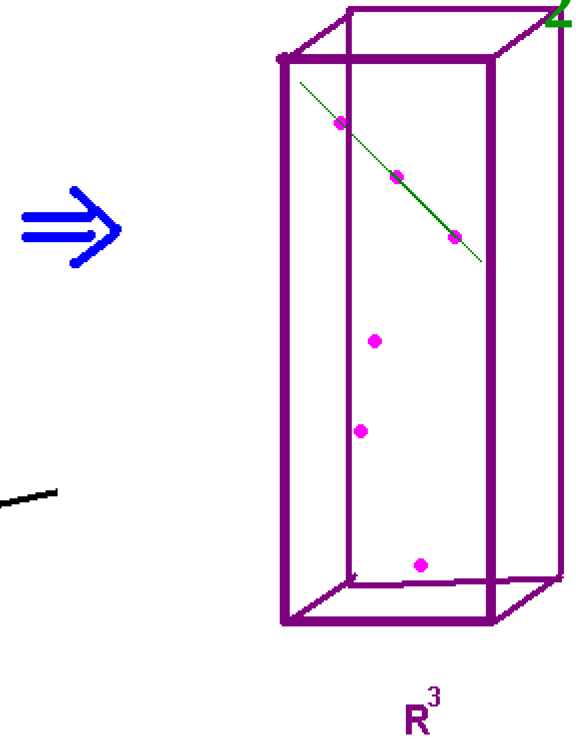
($S_\ell \subseteq \mathcal{V}$ linear algebraic *simplexes*)

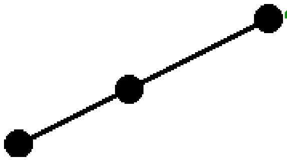


2'nd version



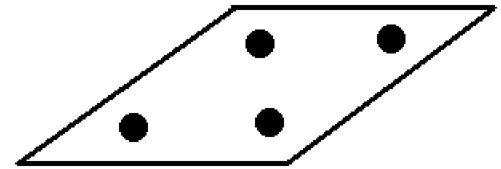


Alternatively: $S_a = \{s_1, ..., s_k\}$ is an *affine* simplex $\Longleftrightarrow$ $S_\ell = \{\underline{s}_2 - \underline{s}_1,\ \underline{s}_3 - \underline{s}_1,\ \ldots\ , \underline{s}_k - \underline{s}_1\}$ is a *linear algebraic* simplex (any $s_1 \in S_a$) .



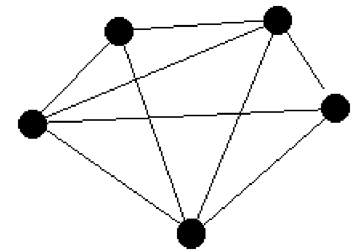
<u>Definition:</u> **(affine) simplexes** in $\mathbf{R}^3$ are

i) 3 colinear points,

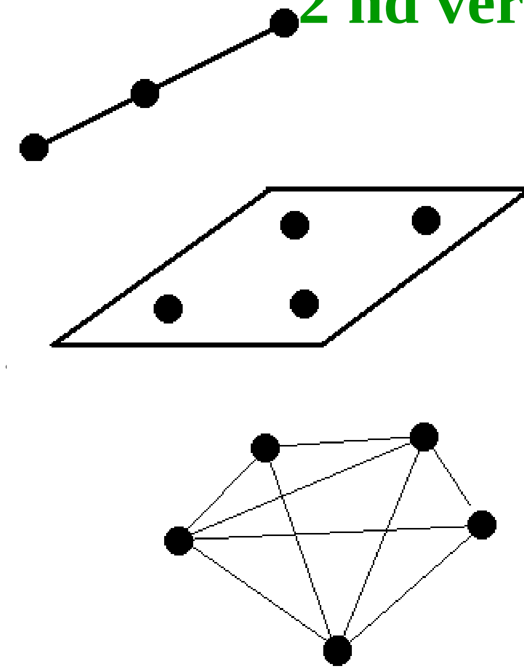


ii) 4 coplanar, no three colinear,

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



2'nd version



<u>Definition:</u> (affine) simplexes in $\mathbf{R}^3$ are

i) 3 colinear points,

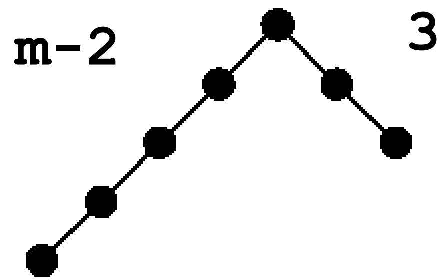
ii) 4 coplanar, no three colinear,

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

Definition: $S_a \subset \mathbb{R}^{D-1}$ is an <u>*affine simplex*</u> if $3 \leq |S_a|$,
S_a is *contained* in a $(|S_a| - 2)$-dimensional hyperplane
but no proper subset $S' \subsetneq S_a$ is *contained*
in a hyperplane of dimension $|S'| - 2$.

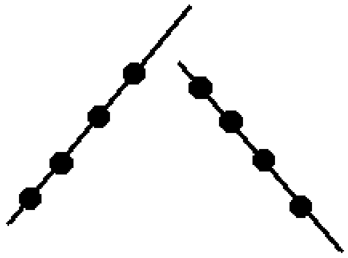
Theorem 3 [1998] (Laflamme-Szalkai) *For* $H \subset \mathbf{R}^3$

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



Theorem 4 [2010] (Balázs Szalkai - I.Szalkai) *For* $H \subset \mathbf{R}^4$

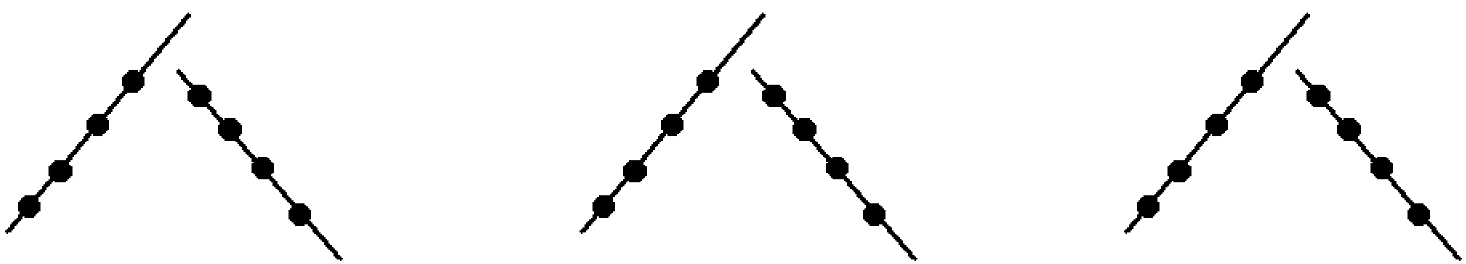
$$\binom{\lfloor m/2 \rfloor}{3} + \binom{\lceil m/2 \rceil}{3} \le simp(\mathcal{H})$$



Mostly contain (affine) simplexes of three points.

General Conjecture **(1998)** (Laflamme, Meng, Szalkai)
no parallel => **the only minimal configurations in R^n are:**

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

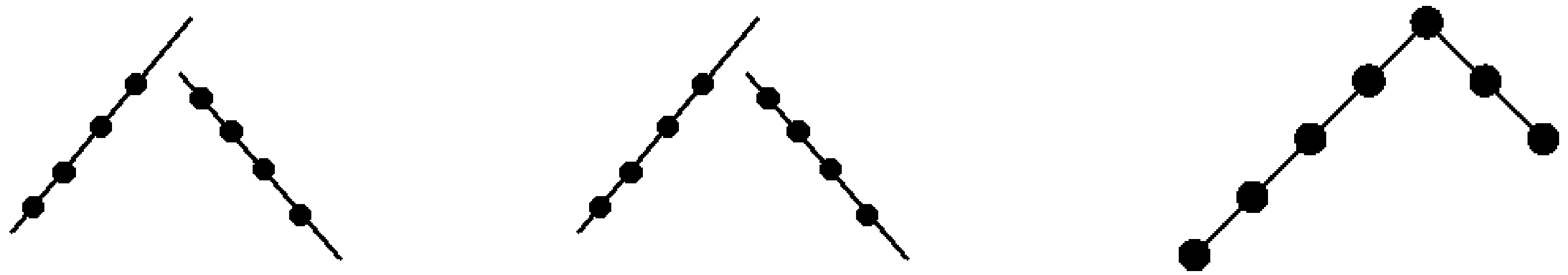


$[\underline{u}_1, \underline{u}_2]$ $[\underline{u}_3, \underline{u}_4]$ . . . $[\underline{u}_i, \underline{u}_{i+1}]$ . . . $[\underline{u}_{n-1}, \underline{u}_n]$

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

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

? 2) *If* n *is odd* => H *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.* □



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

2'nd version

***New:* no three points are collinear** (or: $k \leq |S|$)

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Definition: $S_a \subset \mathbb{R}^{D-1}$ is an <u>*affine simplex*</u> if $3 \le |S_a|$,
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***k = d := D*-1**

Remark: Two kinds of subsets of $\mathcal{H}$ 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 $d - 1$.

2'nd version

Zs.Tuza, I.Szalkai (2014)

Theorem 3 $\forall d \geq 3 \;\; \exists c_d$ *constant:*

If $\mathcal{H} \subset \mathbb{R}^d$, $|\mathcal{H}| = n$ *and*

no d *points from* $\mathcal{H}$ *lie on a hyperplane*

of dimension $d - 2$,

then $\binom{n}{d+1} - c_d \cdot n^d \leq simp_a(\mathcal{H})$.

Corollary 4 *For* $\mathcal{H} \subset \mathbb{R}^3$, $|\mathcal{H}| = n$,

no three collinear

$\binom{n}{4} - O(n^3) \leq simp_a(\mathcal{H})$ *as* $n \to \infty$.

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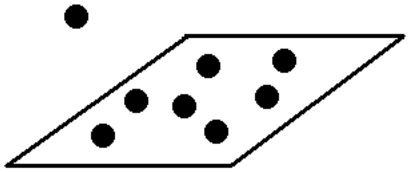

$\binom{n}{4} - O(n^3) \leq simp_a(\mathcal{H})$ *as* $n \to \infty$.

(asymptotically tight)

Proposition 7 *There is an arrangement of n points in $\mathbb{R}^3$, such that the number of affine simplexes determined by them is only*

$$\binom{n-1}{4} - \frac{(n-2)(n-5)}{2} \qquad \text{if } n \text{ is even,}$$

$$\binom{n-1}{4} - \frac{(n-3)(n-5)}{2} \qquad \text{if } n \text{ is odd;}$$

that is, $\frac{1}{24}n^4 - \frac{5}{12}n^3 + O(n^2)$.

Combinatorial formulation

Definition 5 *A hypergraph* $\mathcal{H} = (X, \mathcal{E})$ *is* q-***linear*** *(*$q \geq 1$*)* *if* $|E' \cap E''| < q$ *for all* $E', E'' \in \mathcal{E}$, $E' \neq E''$. $\square$

E.g. in a 1-linear hypergraph any two edges are disjoint,
"2-linear" coincides with "linear" hypergraphs in the usual sense
(in Euclidean spaces any two points uniquely determine a line).

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E.g. in a 1-linear hypergraph any two edges are disjoint, "2-linear" coincides with "linear" hypergraphs in the usual sense (in Euclidean spaces any two points uniquely determine a line).

$\binom{H}{k} = \{\ k$ -element subsets of $H\ \}$,

$\mathcal{E}_k := \bigcup_{E \in \mathcal{E}} \binom{E}{k}$; $(X, \mathcal{E}_k)$ is the k-**section hypergraph** of $\mathcal{H}$,

$\mathcal{E}^0_{k+1} := \{F \in \binom{X}{k+1} \mid \binom{F}{k} \cap \mathcal{E}_k = \emptyset\}$.

members of $\mathcal{E}_k \cup \mathcal{E}^0_{k+1}$ are the $(k-1)$-dimensional **semi-simplexes** in $\mathcal{H}$ $(k = d+1)$

2'nd version

Zs.Tuza, I.Szalkai (2014)

Theorem 6 *For $k \geq 3$ there is a constant $c = c_k$ such that*

$$|\mathcal{E}_k| + |\mathcal{E}^0_{k+1}| \geq \binom{n}{k} - cn^{k-1}$$

for all $(k-1)$ -linear hypergraphs $\mathcal{H} = (X, \mathcal{E})$, $|X| = n$. $\square$

This result implies Theorem 3.

2'nd version

Sperner families

For any $\mathcal{H} = (X, \mathcal{E})$ (not necessarily q-linear) and k

$\mathcal{S}_k(\mathcal{H}) := \mathcal{E}_k \cup \mathcal{E}^0_{k+1}$ is a **Sperner family,**

YBLM inequality[2]

$$\sum_{S \in \mathcal{S}} \binom{n}{|S|}^{-1} \leq 1$$

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Yamamoto [1954], **B**ollobás [1965], **L**ubell [1966], **M**eshalkin [1963]

$\Rightarrow$ Hungarian architect **Ybl M**iklós (1814-1891)

https://en.wikipedia.org/wiki/Mikl%C3%B3s_Ybl

2'nd version

Sperner families

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YBLM inequality[2]

$$\sum_{S \in \mathcal{S}} \binom{n}{|S|}^{-1} \leq 1$$

we let

$$s(n,k) := \min_{\mathcal{H} \text{ is } \underline{(k-1)\text{-linear},}\ |X|=n} \sum_{S \in \mathcal{S}_k(\mathcal{H})} \binom{n}{|S|}^{-1}$$

$$s'(n,k) := \min_{\mathcal{H}=(X,\mathcal{E}),\ |X|=n} \sum_{S \in \mathcal{S}_k(\mathcal{H})} \binom{n}{|S|}^{-1}$$

2'nd version

Zs.Tuza (2014)

Theorem 8 *For every fixed* $k \geq 2$*, the limits*

$$s_k := \lim_{n\to\infty} s(n,k) \qquad \text{and} \qquad s'_k := \lim_{n\to\infty} s'(n,k)$$

exist and satisfy

$$0 < s'_k \leq s_k < 1$$

strict inequality at both ends.

Turán numbers

For fixed k-uniform hypergraph $\mathcal{F}$

$ex(n, \mathcal{F})$:= Turán number = the *maximum number of edges* in a k-uniform hypergraph of order n which does not contain any subhypergraph isomorphic to $\mathcal{F}$.

Turán numbers

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$\mathcal{K}_{k+1}^{(k)} := (X_k, \mathcal{E}_k)$, $|X_k| = k+1$, $|E| = k$ for $E \in \mathcal{E}$

(=the complete k-uniform hypergraph of order k).

E.g. $\mathcal{K}_3^{(2)} = K_3$, $ex(n, K_3) = \left\lfloor \frac{n^2}{4} \right\rfloor$ well known,

for $2 < k$ $ex(n, \mathcal{K}_{k+1}^{(k)})$ is *open*.

Remark12 *If* $\mathcal{H} = (X, \mathcal{E})$ *is a* k*-uniform hypergraph of order* n *such that each* $(k+1)$*-tuple of vertices contains at least one edge of* $\mathcal{H}$*, then* $\mathcal{E}^0_{k+1} = \emptyset$.

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In particular, taking $\mathcal{H}$ *as the complement of a hypergraph extremal for* $ex(n, \mathcal{K}^{(k)}_{k+1})$*, we obtain:*

$$s'(n,k) \leq 1 - \frac{ex(n, \mathcal{K}^{(k)}_{k+1})}{\binom{n}{k}} \qquad \text{and} \qquad s'_k \leq 1 - \lim_{n\to\infty} \frac{ex(n, \mathcal{K}^{(k)}_{k+1})}{\binom{n}{k}} \qquad .$$

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Hence, any lower bound on the Turán density of $\mathcal{K}^{(k)}_{k+1}$ *implies an upper bound on* s'_k*.*

IX.
General Hierarchy

On the Mathematical Foundation of Reaction Mechanisms

(manuscript in preparation, 130611)

Peter H.Sellers, ✠2014 , Árpád Pethő,Á. ✠2012

István Szalkai

Definitions

A chemical (stoichiometric) system is made up of an infinite hierarchy of *disjoint finite sets*:

Definition 2 *We introduce the (arbitrary)* nonempty disjoint finite sets *sets* $\mathcal{A}_x$ *for* $x = 0, 1, ... \in \mathbb{N}$ *as* ($\mathcal{A}, \mathcal{M}, \mathcal{E}, \mathcal{C}$ *are special notations for* $\mathcal{A}_0, ..., \mathcal{A}_3$)*:*

o) $\mathcal{A} := \mathcal{A}_0 = \{A_1, ..., A_a\}$ *called* ***atoms,***

i) $\mathcal{M} := \mathcal{A}_1 = \{M_1, ..., M_m\}$ *called* ***molecules*** *or* ***species,***

ii) $\mathcal{E} := \mathcal{A}_2 = \{E_1, ..., E_e\}$ *called* ***elementary mechanistic steps*** *or* ***reactions,***

iii) $\mathcal{C} := \mathcal{A}_3 = \{C_1, ..., C_c\}$ *called (elementary)* ***mechanisms*** *or* ***catal-izatinos,***

...

x) $\mathcal{A}_x = \left\{A_1^{(x)}, ..., A_{d(x)}^{(x)}\right\}$ *called the* x ***-th level of hierarchy,*** ... . □

Definition 3 *We define the* ***algebras*** $\mathcal{L}_x := (L_x, +, \cdot)$ *for* $x = 0, 1, ... \in \mathbb{N}$ *as the ground sets*

$$L_x := \left\{ \sum_{j=1}^{d(x)} \alpha_j \cdot A_j^{(x)} : \alpha_j \in \mathbb{Z} \right\} \ , \tag{3}$$

abbreviating $\sum_{j=1}^{d(x)} \alpha_j \cdot A_j^{(x)}$ *as* $\left[\alpha_1, ..., \alpha_{d(x)}\right]$ *, equipped with the usual operations*

$$\left[\alpha_1, ..., \alpha_{d(x)}\right] + \left[\beta_1, ..., \beta_{d(x)}\right] := \left[\alpha_1 + \beta_1, ..., \alpha_{d(x)} + \beta_{d(x)}\right] \tag{4}$$

and

$$\lambda \cdot \left[\alpha_1, ..., \alpha_{d(x)}\right] := \left[\lambda \cdot \alpha_1, ..., \lambda \cdot \alpha_{d(x)}\right] \quad \text{for } \lambda \in \mathbb{Z} \ . \tag{5}$$

Clearly the ***bases*** *of* $\mathcal{L}_x$ *are the sets* $\mathcal{A}_x$ *.* □

$$\Delta_1(M_j) = \sum_{k=1}^{a} \alpha_{j,k} \cdot A_k \ , \quad \Delta_2(E_i) = \sum_{j=1}^{m} \mu_{i,j} \cdot M_j \quad (1 \le i \le e) \tag{6}$$

as
$$\sum_{j=1}^{m} \mu_{i,j} \cdot \alpha_{j,k} = 0 \quad for\ 1 \le i \le e\ ,\ 1 \le k \le a\ . \tag{7}$$

Using matrices (7) can be written as

$$\left[\mu_{i,j}\right]_{e,m} \cdot \left[\alpha_{j,k}\right]_{m,a} = [0]_{e,a} \ , \tag{8}$$

or in the language of the linear mappings

$$\boxed{\Delta_1 \circ \Delta_2 = O \quad i.e. \quad \mathrm{Im}\,(\Delta_2) \subseteqq Ker\,(\Delta_1)} \tag{9}$$

where, of course

$$\Delta_2 : \mathcal{L}_2 \rightarrow \mathcal{L}_1 \quad and \quad \Delta_1 : \mathcal{L}_1 \rightarrow \mathcal{L}_0\ . \tag{10}$$

($\left[\mu_{i,j}\right]_{e,m}$ is called *stoichiometric* while $\left[\alpha_{j,k}\right]_{m,a}$ is the *composition matrix.*)

in general:

Definition 4 *For* $x \in \mathbb{N}$, $x \neq 0$ *we call the linear mappings*

$$\Delta_x : \mathcal{L}_x \to \mathcal{L}_{x-1} \tag{11}$$

stoichiometric connections *between* $\mathcal{L}_x$ *and* $\mathcal{L}_{x-1}$ *if*

$$\Delta_x \circ \Delta_{x+1} = O \qquad \textit{for} \quad x = 1, 2, \ldots \tag{12}$$

where $O = O_x : \mathcal{L}_{x+1} \to \mathcal{L}_{x-1}$ *is the* null-mapping. □

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Remark 5 *The requirement (12) can be written equivalently as*

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Definition 6 *We call a system of algebras and mappings*

$$\mathcal{H} = (\mathcal{L}_x, \Delta_{x+1} : x \in \mathbb{N}) \tag{14}$$

(stoichiometric) hierarchy*, if it satisfies Definitions 2 through 4.* □

Properties

For $\underline{v} = \sum_{j=1}^{d(x)} \alpha_j \cdot A_j^{(x)} \in L_x$ $(0 < x)$, $\underline{v} \in Ker\,(\Delta_x)$ we know that

$$\Delta_x\,(\underline{v}) = \sum_{j=1}^{d(x)} \alpha_j \cdot \Delta_x \left(A_j^{(x)} \right) = \sum_{j=1}^{d(x)} \alpha_j \cdot \left(\sum_{i=1}^{d(x-1)} \beta_i^{(j)} \cdot A_i^{(x-1)} \right)$$

$$= \sum_{i=1}^{d(x-1)} \left(\sum_{j=1}^{d(x)} \alpha_j \beta_i^{(j)} \right) \cdot A_i^{(x-1)} = \underline{0}$$

which includes $\displaystyle\sum_{j=1}^{d(x)} \alpha_j \beta_i^{(j)} = 0 \quad \text{for} \;\; i \leq d\,(x-1)$

since $\left\{ A_1^{(x)}, ..., A_{d(x)}^{(x)} \right\}$ was assumed to be a base.

above implies

$$\boxed{\mathrm{Im}\,(\Delta_2) = \textit{the set of all balanced reactions.}} \qquad (16)$$

$$\boxed{Ker\,(\Delta_2) = \textit{the set of all cycle-mechanisms.}} \qquad (17)$$

In general

Definition 7 *For* $x > 0$ *the* elements *of*

$Ker\,(\Delta_x)$ *are called* (generalized) ***cycle-mechanisms***

$\mathrm{Im}\,(\Delta_x)$ *are called* ***balanced mechanisms.*** □

Clearly, by (13) each balanced mechanisms must be cycles.

We did *not* prescribe $Ker\,(\Delta_x) = \emptyset$, so we may use

Definition 8 *For $x > 0$ we call the vectors $\underline{w}_1, \underline{w}_2 \in L_x$ to be* ***equivalent*** *modulo $Ker\,(\Delta_x)$ if and only if*

$$\underline{w}_2 - \underline{w}_1 \in Ker\,(\Delta_x) \quad . \tag{18}$$

We shorten

$$\underline{w}_1 \rightleftarrows \underline{w}_2 \quad . \qquad \square \tag{19}$$

Clearly

$$\underline{w}_2 = \underline{w}_1 + \underline{y} \quad \text{for some } \underline{y} \in Ker\,(\Delta_x) \quad . \tag{20}$$

It is well known, that $\rightleftarrows$ is an *equivalence relation* and

$$\boxed{L_x/_{\rightleftarrows} \cong \mathrm{Im}\,(\Delta_x) \ .} \tag{21}$$

Dual mappings $\Delta_x^* : \mathcal{L}_{x-1}^* \to \mathcal{L}_x^* \quad (1 \leq x).$

mathematical definition

Definition 9 *Let V and W be any linear spaces ,* usually $\Gamma = \mathbb{R}$.

(i) *The **dual space** V^* is the set of linear mappings (functions) $f : V \to \Gamma$. The addition and scalar multiplication for $f_1, f_2, f \in V^*$ and $\lambda \in \Gamma$*

$$(f_1 \oplus f_2)(v) \quad : \quad = f_1(v) + f_2(v)$$
$$(\lambda \odot f)(v) \quad : \quad = \lambda \cdot f(v) \qquad (v \in V, \ \lambda \in \Gamma). \tag{25}$$

(ii) *For* any *linear mapping $\mathcal{M} : V \to W$, the **dual mapping***

$$\mathcal{M}^* : W^* \to V^* , \quad g \longmapsto f \tag{26}$$

The elements of V^* are called also *functionals* or *valuations.*

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The elements of V^* are called also *functionals* or *valuations.*

Definition 10 *The dual mappings $\Delta_x^* : \mathcal{L}_{x-1}^* \to \mathcal{L}_x^* \quad (1 \le x)$ are called **dual stoichiometric connections.*** □

(the *matrices* of Δ_x^* are the **transposes** of the matrices of Δ_x .)

p. 1 P. H. Sellers, The Rockefeller University
1230 York Ave., N.Y., NY 10021
USA

27 Jan. 2003

Istvan Szalkai
University of Vezprém
P.O. Box 158, Vezprém
Hungary

Dear Istvan,

Thankyou for the e-mail. Let me respond to the comments you have made, based on the POSTSCRIPT in my letter of 11 April 2002. I am thinking of comments 1, 2 and 3, in particular.

(1.) I agree with your suggestion that we focus on the mathematics, i.e. the properties of 3 vector spaces

$$\mathcal{E} \xrightarrow{\Delta_2} \mathcal{M} \xrightarrow{\Delta_1} \mathcal{A}$$

joined by linear transformations such that $\Delta_1(\Delta_2(E)) = 0$ for all $E \in \mathcal{E}$. Let us

X. Valuation Operator

Definition ***6.5.***

(i) *call the elements of an arbitrary set* $\{C_1, \ldots, C_n\}$ ***components,*** *the linear combination* $\underline{S} = \sum_{i=1}^{n} s_i \cdot C_i \; (s_i \in \mathbb{R})$ *(chemical)* ***structures,***

$V := \{\sum_{i=1}^{n} s_i \cdot C_i : s_i \in \mathbb{R}\}$ *are* ***sets of massess.***

(ii) *Any linear functional* $\mathcal{L} : V \to \mathbb{R}$ *is called* ***evaluating operator.*** □

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(ii) Any linear functional $\mathcal{L} : V \to \mathbb{R}$ *is called* ***evaluating operator.*** □

Theorem ***6.6.*** *All the evaluating operators on* V *have the form*

$$\mathcal{L}(\underline{S}) = \sum_{i=1}^{n} a_i \cdot s_i$$

where the coefficient vector $\underline{a} = [a_1, \ldots, a_n]^T \in \mathbb{R}^n$ *is uniquely determined by* $\mathcal{L} : a_i = \mathcal{L}(C_i)$. □

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where the coefficient vector $\underline{a} = [a_1, \ldots, a_n]^T \in \mathbb{R}^n$ *is uniquely determined by* $\mathcal{L}$: $a_i = \mathcal{L}(C_i)$. □

Immediately we get

Theorem 6.7. (Hess' law) *If the reactions* $X_1, \ldots, X_k$ *result the zero mechanism* $\underline{O}$, *then the sum of the heats* $\mathcal{H}(X_1), \ldots, \mathcal{H}(X_k)$ *is* 0. □

The fact $V^* \cong V$ implies

Theorem 77 ***(PhD 6.8.T.)*** *If* V *is built up from* n *components, then there are* at most n *linearly independent evaluating operators* $\mathcal{L}_1, ..., \mathcal{L}_n$ *, so all each other evaluating operator* $\mathcal{L}$ *can be expressed as* $\mathcal{L} = \alpha_1 \mathcal{L}_1 + ... + \alpha_n \mathcal{L}_n$ *.* □

Cauchy-Bunyakowsky-Schwarz's inequality:

Theorem 78 ***(PhD 6.9.T.)*** *For any* V *and* $\mathcal{L} : V \to \mathbb{R}$ *there is a constant* $c \in \mathbb{R}^+$ *such that*

$$| \mathcal{L}(\underline{S}) | \leq c \cdot \|\underline{S}\| \quad \textit{for } \underline{S} \in V \ ,$$

where $\|\underline{S}\| = \sqrt{s_1^2 + \ldots + s_n^2}$, $\quad c = \sqrt{a_1^2 + \ldots + a_n^2}$ □

Theorem 6.10. *If V_1 and V_2 are generated by* $\mathcal{C} = \{C_1, \ldots, C_n\}$ *and* $\mathcal{D} = \{D_1, \ldots, D_m\}$ *resp,* $\mathcal{C} \cap \mathcal{D} = \emptyset$ *and* $V = V_1 \oplus V_2$ *, then V has evaluating operators only:*

$$\mathcal{L} = \mathcal{L}\,|_{V_1} \oplus \mathcal{L}\,|_{V_2}$$

$$\mathcal{L}\,(\underline{S}) = \textstyle\sum_{i=1}^{n} a_i s_i + \sum_{j=1}^{m} b_j t_j \quad \textit{for} \quad \underline{S} = \sum_{i=1}^{n} s_i C_i + \sum_{j=1}^{m} t_j D_j\,.$$

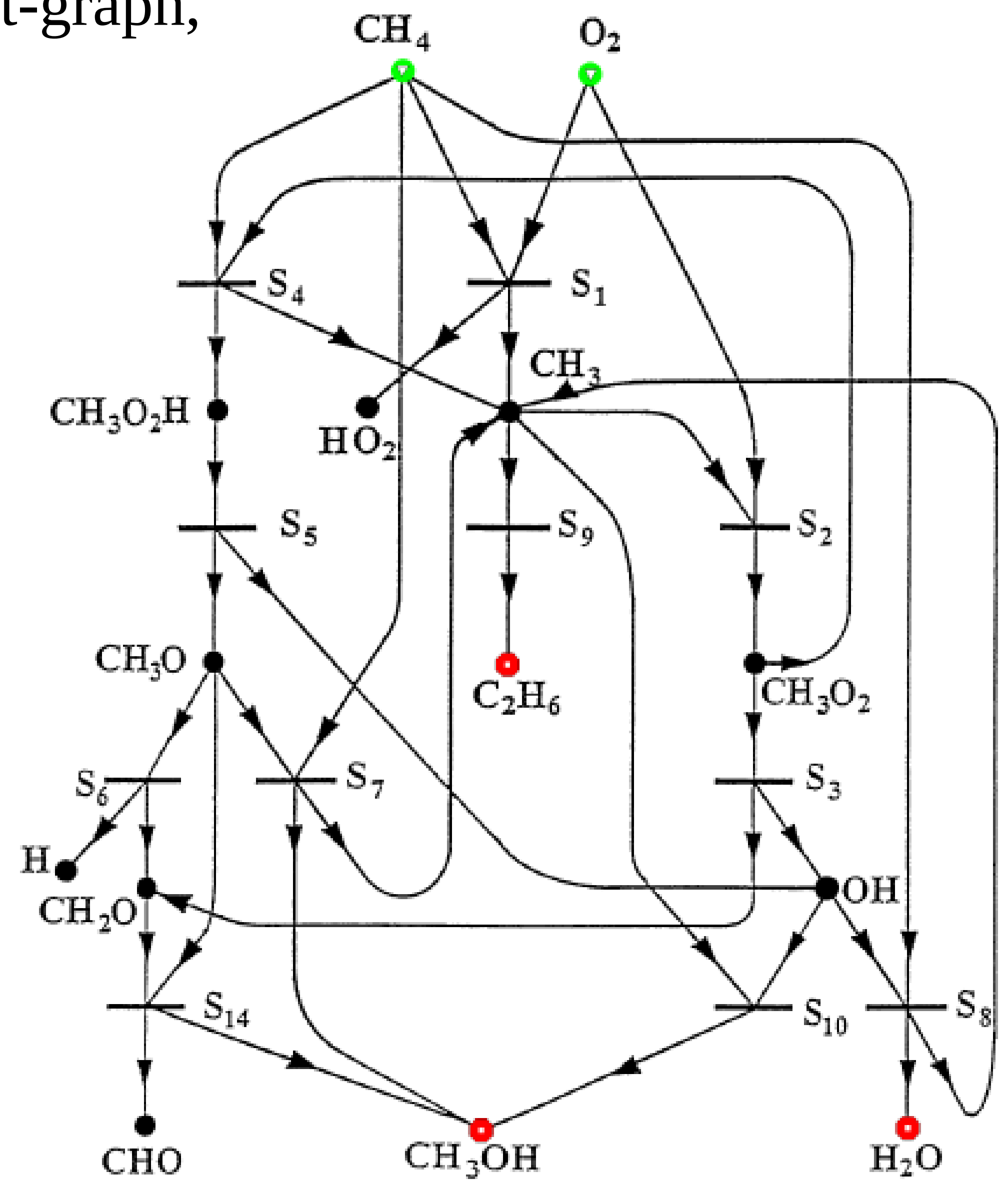
Theorem 6.11. *For any two scalar products* $\mathcal{A}, \mathcal{B} : V \times V \to \mathbb{R}$ *there is an* continuous *automorphism* $\mathcal{I} : V \to V$ *such that*

$$\mathcal{A}(\underline{u}, \underline{v}) = \mathcal{B}(\mathcal{I}(\underline{u}), \mathcal{I}(\underline{v})) \ (\underline{u}, \underline{v} \in V\,). \qquad \square$$

Roughly speaking this means, that all the evaluating operators of a mass-set differ from a scalar multiplier only.

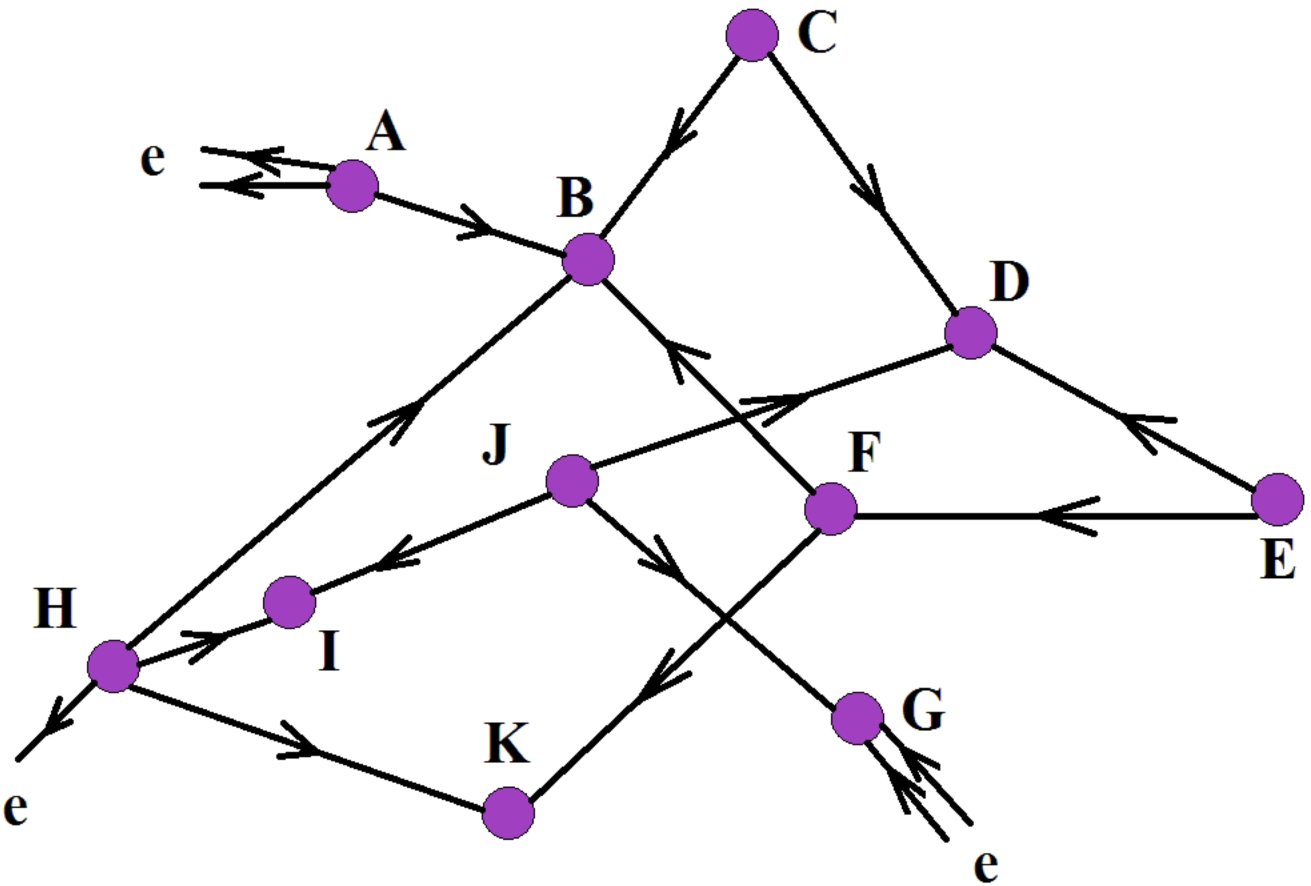
XI.
Graphs

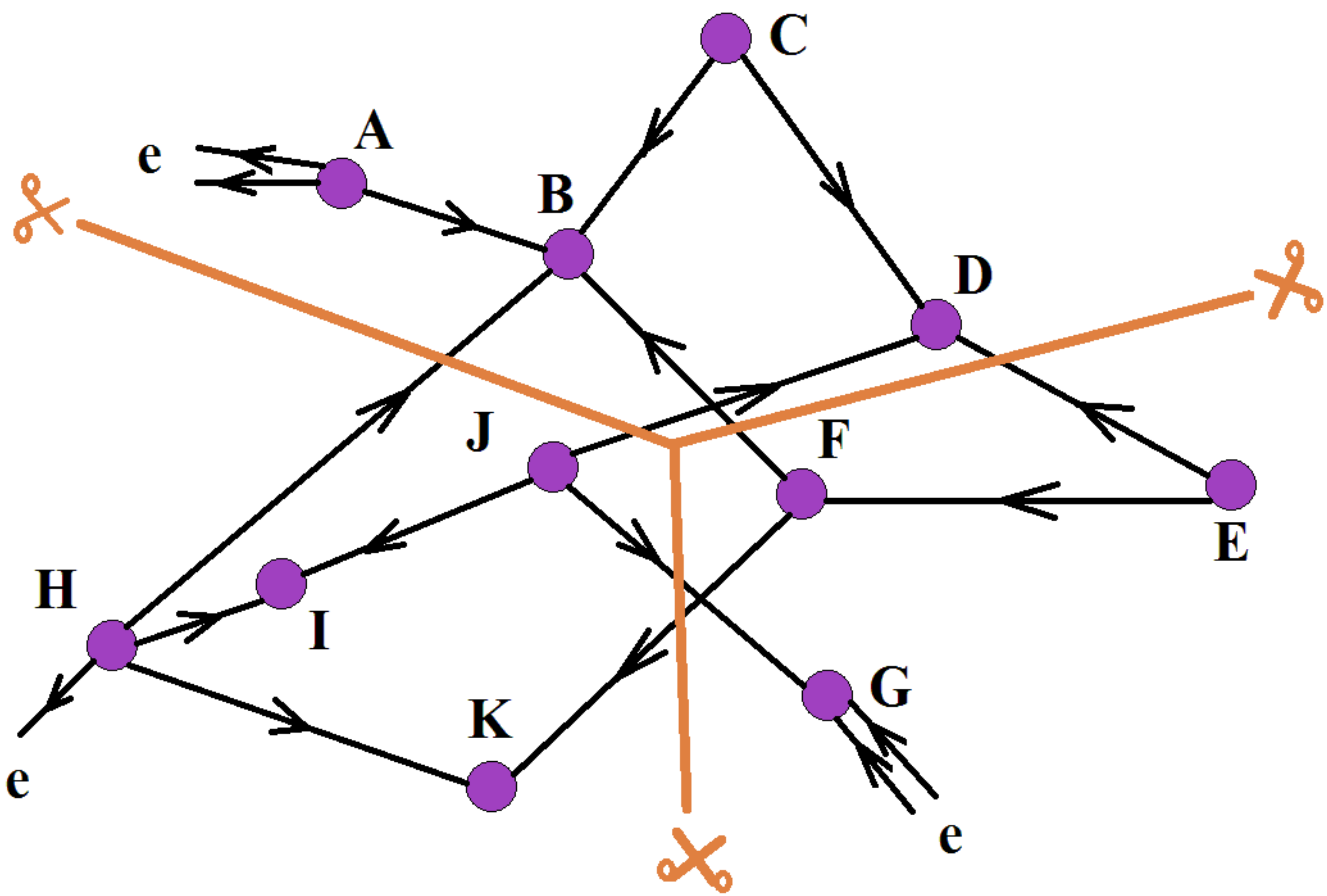
Petri-graph (P-graph), Volpert-graph, Feinberg–Horn–Jackson-graph



Egy P-gráf ([B99])

Dealing with the *chemical structure* (an idea) :

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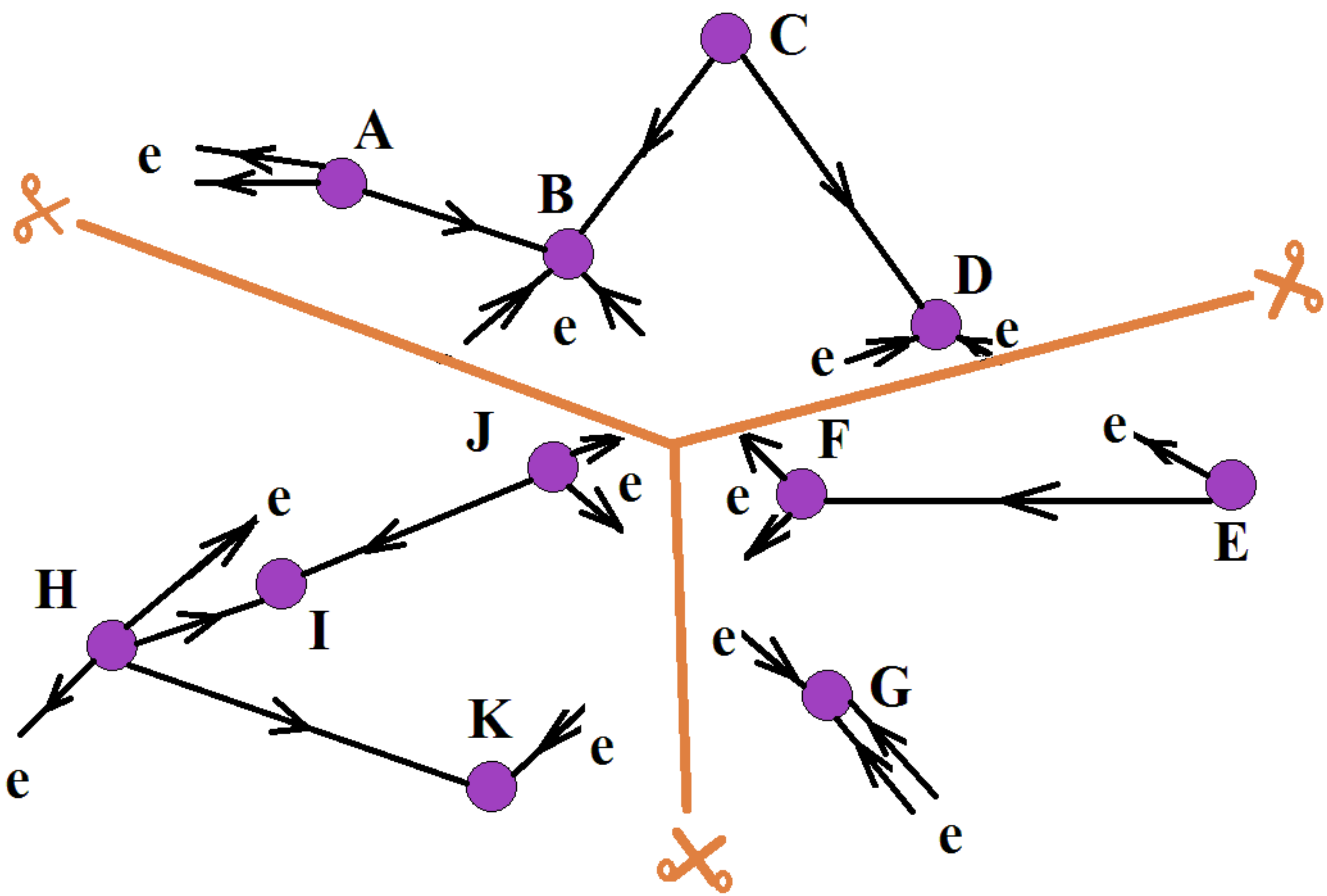
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	A	B	C	D	E	F	G	H	I	J	K	e
A	*	+1										+2
B	−1	*	−1			−1		−1				
C		+1	*	+1								
D			−1	*	−1					−1		
E				+1	*	+1						
F		+1			−1	*					+1	
G							*			−1		−2
H		+1						*	+1		+1	+1
I								−1	*	−1		
J				+1			+1		+1	*		
K						−1		−1			*	
e	−2						+2	−1				*

	A	B	C	D	E	F	G	H	I	J	K	e
A	*	+1										**+2**
B	−1	*	−1									**−2**
C		+1	*	+1								
D			−1	*								**−2**
E					*	+1						**+1**
F					−1	*						**+2**
G							*					**−3**
H								*	+1		+1	**+2**
I								−1	*	−1		
J									+1	*		**+2**
K								−1			*	**−1**
e	**−2**	**+2**		**−2**	**−1**	**−2**	**+3**	**−2**		**−2**	**+1**	*

	A	B	C	D	E	F	G	H	I	J	K	e	
A	*	+1										+2	
B	−1	*	−1			$M^{(1,2)}$			$M^{(1,3)}$			−2	$e^{(1)}$
C		+1	*	+1									
D			−1	*								−2	
E					*	+1						+1	
F		$M^{(2,1)}$			−1	*			$M^{(2,3)}$			+2	$e^{(2)}$
G							*					−3	
H								*	+1		+1	+2	
I		$M^{(3,1)}$				$M^{(3,2)}$		−1	*	−1			$e^{(3)}$
J									+1	*		+2	
K								−1			*	−1	
e	−2	+2		−2	−1	−2	+3	−2		−2	+1	*	

cut

szétvágás:

$$e_j^{(i)\ \acute{U}J} = e_j^{(i)\ R\acute{E}GI} + \sum_{k \neq i} \sum_{\ell} M^{(i,j)}[j, \ell]$$

összeillesztés: $M^{(i,j)} = ?$

glue

Many thanks to

You