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ON MINIMAL SOLUTIONS OF SYSTEMS OF LINEAR EQUATIONS WITH APPLICATIONS

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Abstract. We give a thorough investigation of the structure of solution sets of both homogeneous and inhomogeneous systems of linear equations, from the viewpoint of their *minimal solutions* (which use minimal sets of columns of the coefficient matrix). We also discuss applications in chemistry (stoichiometry).

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1. INTRODUCTION

Systems of linear equations have an enormous amount of applications in many areas of science and technology. For our present research we took chemistry (stoichiometry) as a direct motivation; these applications are outlined in the last section. But beside them and beyond pure theoretical interest, it is plausible to guess that our results can be applied in further areas, too, e.g. in physics (dimensionless groups).

The main targets of our research are the *minimal solutions* of systems of linear equations. We call a solution *minimal* if it uses a minimal set of column vectors of the coefficient matrix; see Definition 1. (The difference and connections between minimal and *base* solutions are explained in Remark 3.)

The structure of the set of minimal solutions is revealed in Proposition 3 and in Propositions 7 through 8, the connection between minimal and other solutions (without any restrictions) is dealt with in Proposition 5 and Theorems 2 and 6.

The results obtained in Theorem 4 and in Theorem 8 have a crucial effect in stoichiometry: all stoichiometrical reactions can be obtained as linear combinations of *minimal* ones. This result could also simplify the research question raised in Section 5 concerning "*The second level*" in the hierarchy of equations.

Some related notions, their combinatorial and geometrical aspects are surveyed in [7].

The sections below give thorough extensions of A. Pethő's results in [3].

2. BASIC PROPERTIES

Let us consider the systems of linear equations

$$A \cdot \underline{x} = \underline{b} \tag{2.1}$$

and

$$A \cdot \underline{x} = \underline{0} \tag{2.2}$$

where $A \in \mathbb{R}^{n \times m}$, $\underline{b} \in \mathbb{R}^n$ are given, and the solution vectors are $\underline{x} \in \mathbb{R}^m$. We investigate the solution sets

$$M_{A,\underline{b}} := \{\underline{x} \in \mathbb{R}^m : A \cdot \underline{x} = \underline{b}\} \tag{2.3}$$

and

$$M_{A,\underline{0}} := \{\underline{x} \in \mathbb{R}^m : A \cdot \underline{x} = \underline{0}\} . \tag{2.4}$$

Clearly the cases $M_{A,\underline{0}} \neq \{\underline{0}\}$ and $\left|M_{A,\underline{b}}\right| > 1$ are the interesting ones.

We denote the column vectors of A by $\underline{a}_1, \underline{a}_2, \ldots, \underline{a}_m \in \mathbb{R}^n$, that is

$$A = \left[\underline{a}_1, \underline{a}_2, \ldots, \underline{a}_m\right] . \tag{2.5}$$

The assumptions below are not only for simplicity, they have real effect in stoichiometry.

Condition 1. It will be assumed that

i) A does not contain parallel column vectors,

especially

ii) A does not contain $\underline{0}$ as a column vector.

In the inhomogeneous case ($\underline{b} \neq \underline{0}$) we also assume that

iii) A does not contain a column vector parallel to $\underline{b}$.

We are interested in the structure of the *sets of column vectors* of A which effectively take part in the equality (2.1).

Definition 1. (i) For any vector $\underline{x} \in \mathbb{R}^m$ we write

$$\operatorname{supp}(\underline{x}) := \{i \leq m : x_i \neq 0\} \tag{2.6}$$

and call it the **support** of $\underline{x}$. (Especially $\operatorname{supp}(\underline{0}) = \varnothing$.)

(ii) For any set of vectors $M \subseteq \mathbb{R}^m$ we say that a *nonzero* vector $\underline{z} \in M$ has **minimal support** for M if the set $\operatorname{supp}(\underline{z})$ is minimal, that is *there exists no* other nonzero vector $\underline{y} \in M$ for which $\operatorname{supp}\left(\underline{y}\right) \subsetneqq \operatorname{supp}(\underline{z})$ holds.

We will call such (nonzero) vectors $\underline{z} \in M$ shortly **minimal** (for M).

(iii) For *any set* of vectors $M \subseteq \mathbb{R}^m$ we denote by $M^{\min}$ the set of all minimal (for M) vectors in M, that is

$$M^{\min} := \left\{\underline{z} \in M : \underline{z} \text{ is minimal}\right\} . \tag{2.7}$$

(iv) Clearly $M^{\min}_{A,\underline{b}}$ and $M^{\min}_{A,\underline{0}}$ stand for the sets of minimal elements in $M_{A,\underline{b}}$ and $M_{A,\underline{0}}$, respectively. We call the vectors in $M^{\min}_{A,\underline{b}}$ and $M^{\min}_{A,\underline{0}}$ the **minimal solutions** of the equalities (2.1) and (2.2).

Clearly, when solving (2.1) or (2.2), we only need those column vectors of A which correspond to $\operatorname{supp}(\underline{x})$. This is discussed in details in Definition 2 and Proposition 5 below.

We explain the difference between the popular *base solutions* and our *minimal solutions* in Remark 3.

The following observations are obvious; we extensively use them later without further mentioning.

Proposition 1. *For the three parts of Condition 1 the following equivalences hold. Considering the homogeneous equation* (2.2) *we have:*

$$\textbf{i)} \quad \Longleftrightarrow \quad |\operatorname{supp}(\underline{x})| \ge 3 \textit{ for all } \underline{x} \in M_{A,\underline{0}} \setminus \{\underline{0}\}\,,$$

$$\textbf{ii)} \quad \Longleftrightarrow \quad |\operatorname{supp}(\underline{x})| \ge 2 \textit{ for all } \underline{x} \in M_{A,\underline{0}} \setminus \{\underline{0}\}\,.$$

For inhomogeneous equations (2.1) *($\underline{b} \neq \underline{0}$) we have:*

$$\textbf{iii)} \quad \Longleftrightarrow \quad |\operatorname{supp}(\underline{x})| \ge 2 \textit{ for all } \underline{x} \in M_{A,\underline{b}}\,.$$

Proposition 2. *For* any nontrivial *solution* $\underline{x} \in M_{A,\underline{0}}$ *of* (2.2) *there is a* minimal *solution* $\underline{z} \in M^{\min}_{A,\underline{0}}$ *such that*

$$\operatorname{supp}(\underline{z}) \subseteqq \operatorname{supp}(\underline{x})\,. \tag{2.8}$$

The same is valid for (2.1) *with* $\underline{x} \in M_{A,\underline{b}}$ *and* $\underline{z} \in M^{\min}_{A,\underline{b}}$.

Proposition 3. *For any set of vectors* $M \subseteq \mathbb{R}^m$ *the sets* $\operatorname{supp}(\underline{z}) \subseteqq \{1,2,\ldots,m\}$ *for* minimal *vectors* $\underline{z} \in M^{\min}$ *form a* Sperner system*, that is for any two (distinct) minimal vectors* $\underline{z}_1, \underline{z}_2 \in M$ *we have* $\operatorname{supp}(\underline{z}_1) \subsetneqq \operatorname{supp}(\underline{z}_2)$ *and* $\operatorname{supp}(\underline{z}_2) \subsetneqq \operatorname{supp}(\underline{z}_1)$.

We want to extract and investigate the nonzero components of the solution vectors $\underline{x}$ and the corresponding column vectors of A . To simplify our later discussion we introduce one more notion.

Definition 2. For an *arbitrary* vector $\underline{x} \in \mathbb{R}^m$, matrix $A \in \mathbb{R}^{n\times m}$, and set $H \subseteq \{1,\ldots,m\}$ of indices we define the **restrictions** of $\underline{x}$ and A to the set H as

$$\underline{x}\,|_H := [x_i : i \in H] \tag{2.9}$$

and

$$A\,|_H := \left[\underline{a}_i : i \in H\right]\,, \tag{2.10}$$

so $\quad \underline{x}\,|_H \in \mathbb{R}^h \quad$ and $\quad A\,|_H \in \mathbb{R}^{n\times h} \quad$ where $h = |H|$.

We clearly have

Proposition 4. *For* any (fixed) *vector* $\underline{x} \in \mathbb{R}^m$ *the set-function*

$$\begin{aligned} \mu_{\underline{x}} \quad &: \quad \mathcal{P}\{1,\ldots,m\} \longrightarrow \mathbb{R}^n \\ \mu_{\underline{x}} \quad &: \qquad H \qquad \longmapsto (A\,|_H)\cdot(\underline{x}\,|_H) \end{aligned} \tag{2.11}$$

for $H \subseteqq \{1,\ldots,m\}$ *is additive.*

The following correspondence between $\underline{x}\,|_{\mathrm{supp}(\underline{x})}$ and $\underline{x}$ is trivial.

Proposition 5. *If* $\underline{x} \in \mathbb{R}^m$ *is* any solution *of the equation* $A\cdot\underline{x} = \underline{b}$ *then* $\underline{x}\,|_{\mathrm{supp}(\underline{x})}$ *satisfies the equality*

$$\left(A\,|_{\mathrm{supp}(\underline{x})}\right)\cdot\left(\underline{x}\,|_{\mathrm{supp}(\underline{x})}\right) = \underline{b} \quad . \tag{2.12}$$

On the other hand, for any subset $H \subseteq \{1,\ldots,m\}$ *and solution* $\underline{y} \in \mathbb{R}^h$ *(*$h = |H|$*) of the equality*

$$(A\,|_H)\cdot\underline{y} = \underline{b} \tag{2.13}$$

there is at least one *solution* $\underline{x} \in \mathbb{R}^m$ *of the equation* $A\cdot\underline{x} = \underline{b}$ (2.1) *such that*

$$\underline{y} = \underline{x}\,|_H \quad . \tag{2.14}$$

Especially, supp$(\underline{x}) \subseteqq H$ *can be assumed.*

Note that the solution $\underline{x}$ above is not unique in general.

Proposition 5 will be extended for homogeneous equations in Theorem 2 and for inhomogeneous ones in Theorem 6 below. It is interesting that these results are very different.

3. Homogeneous equations

We start with the extension of Proposition 5 for homogeneous equations.

Theorem 2. *Let* $\underline{z} \in M_{A,\underline{0}}^{\min}$ *be any minimal solution of* (2.2), $\underline{z} \neq \underline{0}$. *Then the equation*

$$\left(A\,|_{\mathrm{supp}(\underline{z})}\right)\cdot\underline{y} = \underline{0} \tag{3.1}$$

for $\underline{y} \in \mathbb{R}^h$ *(*$h = \left|\mathrm{supp}\left(\underline{z}\right)\right|$*) has* the only *solutions*

$$\underline{y} = \lambda\cdot\underline{z}\,|_{\mathrm{supp}(\underline{z})} \tag{3.2}$$

where $\lambda \in \mathbb{R}$ *is any number.*

Proof. Clearly $\underline{y}_1 := \underline{z}\,|_{\mathrm{supp}(\underline{z})} \in \mathbb{R}^h$ is a solution of (3.1), in which no coordinate is 0 . Let further $\underline{y}_2 \in \mathbb{R}^h$ be any nontrivial solution of (3.1), *distinct* from $\lambda\cdot\underline{z}$ for all $\lambda \in \mathbb{R}$. Since $\underline{y}_2 \neq \underline{0}$, the ith coordinate of $\underline{y}_2$ is nonzero for some $i \in \mathrm{supp}\left(\underline{z}\right)$, so we can find some $\nu \in \mathbb{R}$ such that the ith coordinate of the vector

$$\underline{z}_2 := \underline{y}_1 - \nu\cdot\underline{y}_2$$

is zero.

If $\underline{z}_2 = \underline{0}$ then $\underline{y}_1$ and $\underline{y}_2$ are parallel, i.e. (3.2) holds.

If $\underline{z}_2 \neq \underline{0}$ then $\underline{z}_2 \in \mathbb{R}^h$ has $\operatorname{supp}(\underline{z}_2) \subsetneqq \operatorname{supp}(\underline{z})$ which is a contradiction since $\underline{z}$ was assumed to be minimal. □

Remark 1. We consider the solutions $\underline{x}$ and $\lambda\underline{x}$ **identical** for all $\lambda \in \mathbb{R}$, but throughout our investigation we do *not* call $\underline{0}$ a solution of (2.2). According to Theorem 2 we can say that *the solution* of (3.1), for any minimal $\underline{z} \in M^{\min}_{A,\underline{0}}$, is **unique** (i.e. up to a scalar multiplier).

Our main problem for both homogeneous and inhomogeneous equations $A \cdot \underline{x} = \underline{0}$ and $A \cdot \underline{x} = \underline{b}$ are the same. We first formulate it for the homogeneous case.

Problem 3. Can *all* solutions of the homogeneous equation $A \cdot \underline{x} = \underline{0}$ be generated from the minimal solutions? In other words: does $M^{\min}_{A,\underline{0}} \subset \mathbb{R}^m$ generate $M_{A,\underline{0}}$ with linear combinations?

The inhomogeneous version of this problem will be Problem 7.

Theorem 4. *$M^{\min}_{A,\underline{0}}$ generates $M_{A,\underline{0}}$ for all matrices $A \in \mathbb{R}^{n\times m}$.*

Proof. We have to show that each vector $\underline{x} \in M_{A,\underline{0}}$ (solution of (2.2)) is a linear combination of vectors from $M^{\min}_{A,\underline{0}}$. We proceed by induction on the *size* of $\operatorname{supp}(\underline{x})$; here $\underline{x} \neq \underline{0}$ can clearly be assumed. In the case $\underline{x} \in M^{\min}_{A,\underline{0}}$ we are done.

For $\underline{x} \notin M^{\min}_{A,\underline{0}}$ choose a minimal vector $\underline{z} \in M^{\min}_{A,\underline{0}}$ such that

$$\varnothing \neq \operatorname{supp}(\underline{z}) \subsetneqq \operatorname{supp}(\underline{x}) \ . \tag{3.3}$$

Let $k \in \operatorname{supp}(\underline{z})$ be any index and consider the vector

$$\underline{x}' := \underline{x} - \frac{x_k}{z_k} \cdot \underline{z} \,, \tag{3.4}$$

which is also a solution of (2.2).

By the definition of $\operatorname{supp}(\underline{z})$ we have $z_k \neq 0$, $x'_k = 0$ (i.e. $k \notin \operatorname{supp}(\underline{x}')$), and so

$$\operatorname{supp}(\underline{x}') \subsetneqq \operatorname{supp}(\underline{x}) \ . \tag{3.5}$$

Clearly $\underline{x}' \neq \underline{0}$ since $\underline{x}' = \underline{0}$ would imply $\underline{x} \parallel \underline{z}$ but $\underline{x} \notin M^{\min}_{A,\underline{0}}$ was assumed.

Finally, by the induction hypothesis we know that $\underline{x}'$ is a linear combination of vectors from $M^{\min}_{A,\underline{0}}$. This fact together with (3.4) and $\underline{z} \in M^{\min}_{A,\underline{0}}$ implies that $\underline{x}$ is also a linear combination of minimal vectors. □

The proof given above implies that (the supports of) *all solutions* $\underline{x} \in M_{A,\underline{0}}$ are covered by *minimal* solutions:

$$\operatorname{supp}(\underline{x}) \subseteqq \bigcup \left\{\operatorname{supp}(\underline{z}) : \underline{z} \in M^{\min}_{A,\underline{0}}\right\} \tag{3.6}$$

what does not follow from Proposition 2.

However, not every *column* of the coefficient matrix A takes part in *any* solutions (reactions in stoichiometry); this is explained in the following assertion.

Proposition 6. *For any index $i \leq m$ the column vector $\underline{a}_i$ takes part in some solution $\underline{x} \in M_{A,\underline{0}}$ (that is, $i \in \operatorname{supp}(\underline{x})$) if and only if $\underline{a}_i$ is linearly* dependent *on the other column vectors $\{\underline{a}_1, \ldots, \underline{a}_{i-1}, \underline{a}_{i+1}, \ldots, \underline{a}_m\}$.*

Proof. For any solution vector $\underline{x}$, write the equality $A\underline{x} = \underline{0}$ as

$$x_i \cdot \underline{a}_i = -\sum_{j \neq i} x_j \cdot \underline{a}_j \ . \tag{3.7}$$

The existence of a solution $\underline{x}$ satisfying $i \in supp(\underline{x})$ is equivalent to the solvability of (3.7) with $x_i \neq 0$. This exactly means the dependency of $\underline{a}_i$ on the vectors $\{\underline{a}_1, \ldots, \underline{a}_{i-1}, \underline{a}_{i+1}, \ldots, \underline{a}_m\}$, because $\underline{a}_i \neq \underline{0}$ has been assumed. □

Nonparallel elements of $M_{A,\underline{0}}^{\min}$ can be linearly dependent. One might ask for a base of $M_{A,\underline{0}}^{\min}$; we have not investigated this question yet.

Now we proceed with the investigation of the *inner* structure of the set of minimal solutions.

Proposition 7. *Let $\underline{z} \in M_{A,\underline{0}}^{\min}$, i.e. $\underline{z}$ is a* minimal *solution of the equation $A \cdot \underline{z} = \underline{0}$. Then the set of column vectors $\underline{a}_i$ "used" by $\underline{z}$,*

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

is a minimal *linearly dependent set.*

Proof. $S_{\underline{z}}$ is linearly dependent since $A \cdot \underline{z} = \underline{0}$ is in fact a linear combination of the elements of $S_{\underline{z}}$.

If some proper subset $T \subset S_{\underline{z}}$ was linearly dependent then $\underline{z}$ would not be minimal. □

This result explains the following notion.

Definition 3. A set $S \subset \mathbb{R}^n$ is called a **linear algebraic simplex** if S is minimal (linearly) dependent, that is S itself is dependent but all its proper subsets $T \subset S$ are independent.

Remark 2. The term "simplex" is also used in Euclidian and in affine geometry with different meanings. In the present paper we deal only with linear algebraic ones but always use the attribute "linear" to avoid confusion. Several notions of simplexes and their applications can be found in [7].

Remark 3. Let us now clarify the *difference* between **base solutions** and **minimal solutions** of a system of (linear) equations (2.1) and (2.2).

For *inhomogeneous* equations (2.1) the base solutions correspond to *bases* of A , i.e. r independent column vectors of A where $r = rank(A)$. The coefficients for resulting $\underline{b}$ when using a base are always uniquely determined. So, a base solution is minimal exactly when it is *nondegenerate*.

For *homogeneous* equations (2.2) (according to [3]) the support of a base solution contains a base of A (as in the previous paragraph) plus exactly one from the remaining column vectors of A. So, in the homogeneous case, all base solutions have size exactly $r+1$, contain dependent column vectors of A, but are not necessarily minimal (a simplex). On the other hand, the set of column vectors of A corresponding to the support of a minimal solution always forms a minimal dependent set (a simplex) but may have size less than $r+1$.

The following characterization is fundamental both in theory and in applications of (linear algebraic) simplexes.

Theorem 5. *A (nonempty) set* $S=\{\underline{v}_1,\underline{v}_2,\dots,\underline{v}_k\}\subset\mathbb{R}^n$ *of vectors is a linear algebraic simplex if and only if there exists a linear combination*

$$\gamma_1\underline{v}_1+\gamma_2\underline{v}_2+\cdots+\gamma_k\underline{v}_k=\underline{0}\,, \tag{3.8}$$

and *for* each *linear combination* (3.8) *we must have* $\gamma_i\neq 0$ *for* all $i\leq k$.
Moreover, the linear combination in (3.8) *is unique up to a constant factor; that is, for all linear combinations*

$$\gamma_1'\underline{v}_1+\gamma_2'\underline{v}_2+\cdots+\gamma_k'\underline{v}_k=\underline{0} \tag{3.9}$$

we must have

$$\left[\gamma_1',\gamma_2',\dots,\gamma_k'\right]=\lambda\cdot[\gamma_1,\gamma_2,\dots,\gamma_k] \tag{3.10}$$

for some $\lambda\in\mathbb{R}\setminus\{0\}$.

Proof. The linear combination (3.8) exists since S is dependent. The minimality of S implies $\gamma_i\neq 0$ for all $i\leq k$.

Suppose now that (3.10) does not hold for any $\lambda\in\mathbb{R}$ for the two sequences $[\gamma_1,\gamma_2,\dots,\gamma_k]$ and $\left[\gamma_1',\gamma_2',\dots,\gamma_k'\right]$ satisfying (3.8) and (3.9), respectively. Then the linear combination

$$\gamma_1'\cdot(3.8)-\gamma_1\cdot(3.9)$$

does not contain $\underline{v}_1$, contradicting the minimality of S.

On the other hand, (3.8) implies that S is linearly dependent. Clearly, S is *not* minimal if and only if there is a linear combination (3.8) where $\gamma_i=0$ for some $i\leq k$. So, the uniqueness of (3.8) (in the sense of (3.10)) together with the assumption "$\gamma_i\neq 0$ for all $i\leq k$" ensures that S must be minimal linearly dependent. □

Using the result above, we can sharpen Proposition 5 for *minimal* solutions $\underline{z}\in M_{A,\underline{0}}^{\min}$ as follows. (See also Remark 1.)

Corollary 1. *For any* minimal solutions $\underline{z}$, $\underline{y}\in M_{A,\underline{0}}^{\min}$ *we have*

$$\operatorname{supp}(\underline{z})=\operatorname{supp}\left(\underline{y}\right)\iff\underline{z}\parallel\underline{y}\quad, \tag{3.11}$$

that is each minimal solution $\underline{z}$ is unique *(up to a scalar multiplier) on its support.*

Proof. The statement follows from Theorem 2, Proposition 7 and Theorem 5. □

In Theorem 6 we extend the result above to *inhomogeneous* equations.
Theorem 5 also implies the following property of linear algebraic simplexes.

Proposition 8. *For any two simplexes S_1 and S_2, for which $S_1 \cap S_2 \neq \varnothing$ holds, and for any vector $\underline{w} \in S_1 \cap S_2$ there is a simplex S_3 contained in $(S_1 \cap S_2) \setminus \{\underline{w}\}$:*

$$S_3 \subsetneqq (S_1 \cap S_2) \setminus \{\underline{w}\} . \tag{3.12}$$

In other words, if $\underline{z}_1$, $\underline{z}_2 \in M^{\min}_{A,\underline{0}}$ are two minimal solutions *of the equation $A \cdot \underline{x} = \underline{0}$ (2.2) such that* $\operatorname{supp}(\underline{z}_1) \cap \operatorname{supp}(\underline{z}_2) \neq \varnothing$ *, then for any* $j \in \operatorname{supp}(\underline{z}_1) \cap \operatorname{supp}(\underline{z}_2)$ *one can find a* minimal solution $\underline{z}_3 \in M^{\min}_{A,\underline{0}}$ *for which*

$$j \notin \operatorname{supp}(\underline{z}_3) \subseteq \operatorname{supp}(\underline{z}_1) \cap \operatorname{supp}(\underline{z}_2) \quad . \tag{3.13}$$

Proof. Consider the linear combinations

$$\gamma_1 \underline{v}_1 + \gamma_2 \underline{v}_2 + \cdots + \gamma_k \underline{v}_k = \underline{0} \tag{3.14}$$

and

$$\delta_1 \underline{u}_1 + \delta_2 \underline{u}_2 + \cdots + \delta_\ell \underline{u}_\ell = \underline{0} \tag{3.15}$$

where $S_1 = \{\underline{v}_1, \underline{v}_2, \ldots, \underline{v}_k\}$ and $S_2 = \{\underline{u}_1, \underline{u}_2, \ldots, \underline{u}_\ell\}$. Now, by Theorem 5 we have $\gamma_j \neq 0$ and $\delta_j \neq 0$ (where $\underline{w} = \underline{v}_j = \underline{u}_j$) and so

$$\begin{aligned} & \frac{1}{\gamma_j}\left(\gamma_1 \underline{v}_1 + \gamma_2 \underline{v}_2 + \cdots + \gamma_k \underline{v}_k\right) - \frac{1}{\delta_j}\left(\delta_1 \underline{u}_1 + \delta_2 \underline{u}_2 + \cdots + \delta_\ell \underline{u}_\ell\right) \\ = \ & \underline{w} - \underline{w} = \underline{0} \quad . \end{aligned} \tag{3.16}$$

This means that the set $S_1 \cap S_2 \setminus \{\underline{w}\}$ is linearly dependent, hence it must contain a simplex S_3 . □

4. Inhomogeneous equations

First we extend Proposition 5 and Corollary 1 to inhomogeneous equations.

Theorem 6. *Let $\underline{z} \in M^{\min}_{A,\underline{b}}$ be a* minimal *solution of the* inhomogeneous *equation $A\underline{x} = \underline{b}$ ($\underline{b} \neq \underline{0}$) and let $H := \operatorname{supp}(\underline{z})$. Then the equation*

$$(A\,|_H) \cdot \underline{y} = \underline{b} \tag{4.1}$$

has the unique *solution $\underline{y} = \underline{z}\,|_H$ only.*

Proof. Let $\underline{y_1} := \underline{z}\,|_H \in \mathbb{R}^h \quad (h = |H|)$, in which no coordinate is 0 . Let further $\underline{y_2} \in \mathbb{R}^h$ be any *other* solution of (4.1), assuming that the ith coordinate of $\underline{y}_2$ is nonzero but distinct from the ith coordinate of $\underline{y}_1$ (for some $i \in \operatorname{supp}(\underline{z})$).

It is well-known that for each $\alpha \in \mathbb{R}$ the vectors

$$\underline{v} = \alpha \cdot \underline{y_1} + (1-\alpha) \cdot \underline{y_2} \tag{4.2}$$

satisfy (4.1). By the assumptions above we can choose an α such that the ith coordinate of $\underline{v}$ is equal to 0 . But then $\operatorname{supp}(\underline{v}) \subsetneqq \operatorname{supp}(\underline{z})$, contradicting the minimality of $\underline{z}$. ☐

Second, we extend Problem 3.

Problem 7. Can *all* solutions of the *in*homogeneous equation $A \cdot \underline{x} = \underline{b}$ be generated from the minimal solutions? In other words, does $M^{\min}_{A,\underline{b}}$ generate $M_{A,\underline{b}}$?

We can prove the following result.

Theorem 8. Each *solution vector* $\underline{x} \in M_{A,\underline{b}}$ *can be written as an affine combination of some elements of* $M^{\min}_{A,\underline{b}}$ *plus a solution of the homogeneous equation*

$$\underline{x} = \sum_{i=1}^{I} \alpha_i \underline{z}_i + \underline{y} \qquad \textit{where} \qquad \sum_{i=1}^{I} \alpha_i = 1 \, , \tag{4.3}$$

all $\underline{z}_i \in M^{\min}_{A,\underline{b}}$ *are minimal solutions* ($i = 1, \ldots, I$, $\alpha_i \in \mathbb{R}$)*, and* $\underline{y} \in M_{A,\underline{0}} \cup \{\underline{0}\}$.

Let us emphasize that Theorem 8 extends the well known formula $M_{A,\underline{b}} = \underline{z} + M_{A,\underline{0}}$ for *minimal* solution vectors. Moreover, together with Theorem 4 it implies that $M^{\min}_{A,\underline{b}} \cup M^{\min}_{A,\underline{0}}$ generates $M_{A,\underline{b}}$.

Proof. Let $\underline{x} \in M_{A,\underline{b}}$ be any solution vector. We proceed by induction on the *size* of $\operatorname{supp}(\underline{x})$; $\underline{x} \neq \underline{0}$ can clearly be assumed.

In the case $\underline{x} \in M^{\min}_{A,\underline{b}}$ we are done.

In the case $\underline{x} \notin M^{\min}_{A,\underline{b}}$ choose a minimal vector $\underline{z} \in M^{\min}_{A,\underline{b}}$ such that

$$\operatorname{supp}(\underline{z}) \subsetneqq \operatorname{supp}(\underline{x}) \ . \tag{4.4}$$

Such a $\underline{z}$ does exist since $\underline{x}$ is not minimal *and* $\operatorname{supp}(\underline{x}) \neq \varnothing$.

Subcase a) There exists a $\underline{z} \in M^{\min}_{A,\underline{b}}$ which has an index $k \in \operatorname{supp}(\underline{z})$ such that $z_k \neq x_k$ (and, of course $z_k \neq 0$).

Then consider the vector

$$\underline{x}' := \left(\underline{x} - \frac{x_k}{z_k} \cdot \underline{z}\right) \cdot \frac{1}{1 - \frac{x_k}{z_k}} = \left(\underline{x} - \beta \underline{z}\right) \cdot \frac{1}{1-\beta} \ . \tag{4.5}$$

It is an affine linear combination of $\underline{x}$ and $\underline{z}$, and hence also a solution of $A \cdot \underline{x} = \underline{b}$. Clearly $x'_k = 0$ (i.e. $k \notin \mathrm{supp}\,(\underline{x}')$), so

$$\mathrm{supp}\left(\underline{x}'\right) \subsetneqq \mathrm{supp}\left(\underline{x}\right) \ , \tag{4.6}$$

moreover $\underline{x}' \neq \underline{0}$ by (4.4). Using the induction hypothesis we know that $\underline{x}'$ is an affine linear combination of vectors from $M^{\min}_{A,\underline{b}}$ plus $\underline{y}' \in M_{A,\underline{0}} \cup \{\underline{0}\}$:

$$\underline{x}' = \sum_{i=1}^{I'} \alpha'_i \underline{z}'_i + \underline{y}' \qquad \text{where} \qquad \sum_{i=1}^{I} \alpha_i = 1 \, . \tag{4.7}$$

From (4.5) and (4.7) we get

$$\underline{x} = (1-\beta)\,\underline{x}' + \beta \underline{z} = (1-\beta) \sum_{i=1}^{I'} \alpha'_i \underline{z}'_i + \beta \underline{z} + (1-\beta)\,\underline{y}' \tag{4.8}$$

which is also an affine linear combination of vectors from $M^{\min}_{A,\underline{b}}$ plus one from $M_{A,\underline{0}} \cup \{\underline{0}\}$.

Subcase b) We have

$$\underline{x}\;|_{\mathrm{supp}(\underline{z})} = \underline{z}\;|_{\mathrm{supp}(\underline{z})} \tag{4.9}$$

for all vectors $\underline{z} \in M^{\min}_{A,\underline{b}}$ satisfying (4.4).

Let $\underline{z} \in M^{\min}_{A,\underline{b}}$ be such a fixed vector. By (4.9) and Proposition 4 we have

$$A|_{\mathrm{supp}(\underline{z})} \cdot \underline{x}|_{\mathrm{supp}(\underline{z})} = A|_{\mathrm{supp}(\underline{z})} \cdot \underline{z}|_{\mathrm{supp}(\underline{z})} = \underline{b} \tag{4.10}$$

and so

$$\left(A|_{\mathrm{supp}(\underline{x})\setminus\mathrm{supp}(\underline{z})}\right) \cdot \left(\underline{x}|_{\mathrm{supp}(\underline{x})\setminus\mathrm{supp}(\underline{z})}\right) = \underline{0} \, . \tag{4.11}$$

Letting

$$\underline{y} := \underline{x}|_{\mathrm{supp}(\underline{x})\setminus\mathrm{supp}(\underline{z})} \tag{4.12}$$

we have $\underline{y} \in M_{A,\underline{0}} \cup \{\underline{0}\}$, and by

$$\mathrm{supp}\left(\underline{z}\right) \cap \mathrm{supp}\left(\underline{y}\right) = \varnothing \tag{4.13}$$

we obtain $\underline{x} = \underline{z} + \underline{y}$ which clearly justifies (4.3) and proves the theorem. □

5. The second level

Recall that the set of solution vectors of the linear equation (2.2) is denoted by $M_{A,\underline{0}}$ in (2.4). Since $M_{A,\underline{0}} \subseteq \mathbb{R}^m$, we can pick some *arbitrary* elements

$$\underline{X}_1, \ldots, \underline{X}_k \in M_{A,\underline{0}} \tag{5.1}$$

and consider the new linear equation

$$\sum_{\ell=1}^{k} m_\ell \underline{X}_\ell = \underline{0} \tag{5.2}$$

for the unknowns.

This is the second step of the **Hierarchy of equations**: the coefficients $\underline{X}_\ell$ of the equality (5.2) are, in fact, all the solutions of the previous (original) equality (2.2).

The final *connection* among the coefficients $\underline{A}_j$ of (2.2) and the solutions $M := [m_1, \ldots, m_\ell]$ of (5.2) has been raised but not investigated yet.

Considering the result of Theorem 4 we could choose $\underline{X}_1, \ldots, \underline{X}_k$ to be all the *minimal* solutions of the (original) equality (2.2).

The stoichiometrical importance of this question will be explained in the next section.

6. Chemical applications

As usual, we consider the reactions in stoichiometry as (systems of) homogeneous linear equations. For example the chemical reaction

$$NaOH + HNO_3 = NaNO_3 + H_2O \tag{6.1}$$

corresponds to the vector-equation

$$[1,0,1,1]^T + [1,1,0,3]^T = [0,1,1,3]^T + [2,0,0,1]^T \tag{6.2}$$

using the base $B = \{H, N, Na, O\}$.

In a general formulation, if the chemical compounds $A_1, A_2, \ldots, A_m$ consist of elements $E_1, E_2, \ldots, E_n$ as $A_j = \sum_{i=1}^{n} a_{i,j} E_i$ ($a_{i,j} \in \mathbb{N}$, $j = 1, 2, \ldots, m$) and we write $\underline{A}_j$ for the vector $\left[a_{1,j}, \ldots, a_{n,j}\right]^T$, then there may exist a chemical reaction between the compounds $\{A_j : j \in S\}$ for any $S \subsetneqq \{1, 2, \ldots, m\}$ if and only if the homogeneous linear equation

$$\sum_{j \in S} x_j \underline{A}_j = \underline{0} \tag{6.3}$$

has a nontrivial solution for some $x_j \in \mathbb{R}$ ($j \in S$), that is if the vector set $\{\underline{A}_j : j \in S\}$ is *linearly dependent*. Similarly, the inhomogeneous linear equation

$$\sum_{j \in S} x_j \underline{A}_j = \underline{b} \tag{6.4}$$

corresponds to the chemical reaction resulting the compound $B = \sum_{i=1}^{n} b_i E_i$ denoted by $\underline{b} = [b_1, \ldots, b_n]^T$. (Of course the reactions obtained in the way described above are only *possibilities*, e.g. the reaction $2Au + 6HCl \to 2AuCl_3 + 3H_2$ does not occur under normal conditions.)

These ideas motivate the study of the objects (2.1) through (2.7). The question "*are there $\underline{A}_i$ and $\underline{A}_j$ parallel for some $i \neq j$?*" (Condition 1.i) means "*are the* *compounds A_i and A_j isomers or multiple doses of each other*?" in the language of stoichiometry.

The *support* of a solution vector $\underline{x} \in \mathbb{R}^m$ (see Definition 1) collects the compounds which effectively take part in the reaction (6.3) or (6.4): $\operatorname{supp}(\underline{x}) \subseteqq S$ in (6.3) and in (6.4). Minimal solution vectors $\underline{x} \in M^{\min}_{A,\underline{b}}$ and $\underline{x} \in M^{\min}_{A,\underline{0}}$ clearly mean *minimal chemical reactions* in the following sense.

Definition 4. The reaction in (6.3) is called a **minimal reaction** if for no $T \subsetneqq S$ might there be any reaction among the compounds $\{A_j : j \in T\}$; that is if the vector set $\{\underline{A}_j : j \in T\}$ is *linearly independent* for any $T \subsetneqq S$.

As Proposition 7 and Definition 3 explain, minimal chemical reactions correspond to minimal linearly dependent sets of vectors, which we call (algebraic) simplexes. Simplexes are widely used e.g. in stoichiometry when finding minimal reactions and mechanisms or for finding *dimensionless groups* in dimensional analysis, see e.g. [1], [4] and [6]. Algorithmic and extremal quantitative questions of minimal reactions (simplexes) were extensively studied in several papers of the authors; we refer only to [9], [2] and [8]. Other kinds of simplexes and their several mathematical aspects are surveyed in [7].

In the present paper we focused on the *inner structure* of $M_{A,\underline{0}}$ and $M_{A,\underline{b}}$, the set of *all* reactions / solutions of the linear equations

$$\sum_{j=1}^{m} x_j \underline{A}_j = \underline{0}\,, \quad \textit{equivalently} \quad A \cdot \underline{x} = \underline{0} \tag{6.5}$$

and

$$\sum_{j=1}^{m} x_j \underline{A}_j = \underline{b}\,, \quad \textit{equivalently} \quad A \cdot \underline{x} = \underline{b} \tag{6.6}$$

i.e. of (2.2) and (2.1)). We gave thorough extensions of the results in [3].

Proposition 5 and its extensions, Theorems 2 and 6 prove the *uniqueness* of the reactions (solutions) in the sense of Remark 1, if the given set of compounds is minimal.

Theorems 4 and 8 are fundamental in our investigations, since they ensure: *All reactions can be obtained from minimal ones*.

Our further results were listed in Remark 3 through Proposition 8.

The "second level of hierarchy" corresponds to **mechanisms**: *sequences of reactions*, i.e. linear combinations of solution vectors of (6.5) (of (2.1) and (2.2)). This and other questions are planned to discuss in [5].

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