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Construction of normal discrete velocity models of the Boltzmann equation

M. C. Vinerean, Å. Windfäll and A. V. Bobylev
Karlstad University - 651 88 Karlstad, Sweden

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Summary. — Discretization methods have been developed on the idea of replacing the original Boltzmann equation (BE) by a finite set of nonlinear hyperbolic PDEs corresponding to the densities linked to a suitable finite set of velocities. One open problem related to the discrete BE is the construction of normal (fulfilling only physical conservation laws) discrete velocity models (DVMs). In many papers on DVMs, authors postulate from the beginning that a finite velocity space with such properties is given and after that study the discrete BE. Our aim is not to study the equations for DVMs, but to discuss all possible choices of finite sets of velocities satisfying this type of restrictions. Using our previous results, *i.e.* the general algorithm for the construction of normal discrete kinetic models (DKMs), we develop and implement an algorithm for the particular case of DVMs of the BE and give a complete classification for models with small number n of velocities ($n \leq 10$).

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1. – Introduction

In this paper, we discuss a general problem related to spurious conservation laws for discrete velocity models (DVMs) of the classical (elastic) Boltzmann equation (BE). This problem is well known, models with spurious conservation laws appeared already at the early stage of the development of discrete kinetic theory [1, 2]. Making a transition from the Boltzmann equation to its discrete version, we often gain some unphysical (spurious) conservation laws. The well-known theorem of uniqueness of collision invariants [3] for the "continuous" velocity space $\mathbb{R}^d$ very often does not work for a finite set of discrete velocities. In 1985, Cercignani introduced [3] the word "normal" for DVMs, which do not have unphysical conservation laws. This terminology became standard and we use it in this paper. Such a condition is usually assumed in most of the mathematical papers on DVMs (see for review [2], and also more recent works like [4, 5]). The progress in the construction of normal models was relatively slow. The inductive method of 1-extensions was proposed in [6] and proved in [7, 8]. A practical criterion for "normality" was also found [9]. However, these were some particular results which did not answer many questions. In particular, it was not clear how to construct all normal DVMs with given number of velocities, what sort of general classification can be introduced for such models, etc. We addressed these and similar questions in our recent publications [10, 11]. The main goal of this paper is to address all questions related to classical DVMs without trying to consider any generalizations. Most of our results (a complete description of normal DVMs with small number of velocities) are obtained for the plane case. Similar problems in $3d$ still remain unclear. However, our method can also be used in this case.

2. – Statement of the problem

We consider below the case of the elastic discrete velocity models (DVMs) and the problem of classification and construction of all normal DVMs, when the dimension d and the order n of the model are known. The general DVM of the BE reads [2, 1]

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_i \cdot \frac{\partial}{\partial \mathbf{x}}\right) f_i(\mathbf{x}, t) = Q_i(f) = Q_i(f_1, \ldots, f_n), \quad i = 1, \ldots, n, \tag{1}$$

where $\mathbf{x} \in \mathbb{R}^d$ and $t \in \mathbb{R}_+$ denote the position and the time, respectively, and

$$V = \{\mathbf{v}_1, \ldots, \mathbf{v}_n\} \subset \mathbb{R}^d, \quad d = 2, 3, \ldots \tag{2}$$

denotes a set of n distinct velocities of the model. The functions $f_i(\mathbf{x}, t)$ are understood as spatial densities of particles having velocities $\mathbf{v}_i \in \mathbb{R}^d$. The collision operators $Q_i(f)$ in (1) are given by

$$Q_i(f) = \sum_{j,k,l=1}^{n} \Gamma_{ij}^{kl}(f_k f_l - f_i f_j) \quad \text{for } i = 1, \ldots, n. \tag{3}$$

This means that particles can change their velocities through pair collisions (reactions)

$$(\mathbf{v}_i) + (\mathbf{v}_j) \to (\mathbf{v}_k) + (\mathbf{v}_l) \tag{4}$$

with probabilities Γ_{ij}^{kl}, $1 \le i, j, k, l \le n$, such that $\Gamma_{ij}^{kl} = \Gamma_{ji}^{kl} = \Gamma_{kl}^{ij} \ge 0$, with equality sign unless the conservation laws

$$\mathbf{v}_i + \mathbf{v}_j = \mathbf{v}_k + \mathbf{v}_l, \qquad |\mathbf{v}_i|^2 + |\mathbf{v}_j|^2 = |\mathbf{v}_k|^2 + |\mathbf{v}_l|^2 \tag{5}$$

are satisfied. The elastic collision (4) satisfies $(d + 2)$ scalar conservation laws (one mass, d momentum and one energy), and therefore the four velocities form a rectangle in $\mathbb{R}^d$.

Definition 1. A DVM (1), (3) *is called* normal *if any solution of the equations*

$$\Psi(\mathbf{v}_i) + \Psi(\mathbf{v}_j) = \Psi(\mathbf{v}_k) + \Psi(\mathbf{v}_l), \tag{6}$$

where indexes $(i, j; k, l)$ *take all possible values satisfying* (5)*, is given by*
$\Psi(\mathbf{v}) = a + \mathbf{b} \cdot \mathbf{v} + c|\mathbf{v}|^2$*, for some constants* $a, c \in \mathbb{R}$ *and* $\mathbf{b} \in \mathbb{R}^d$.

A practical criterion of the normality (non-existence of spurious conservation laws) for any given DVM has been devised in [9] and generalized to discrete kinetic models in [10, 11]. Consider an arbitrary DVM and introduce a set of vectors of reactions [9]

$$\boldsymbol{\theta}_{ij}^{kl} = \Big(\ldots, \underset{(i)}{1}, \ldots, \underset{(j)}{1}, \ldots, \underset{(k)}{-1}, \ldots, \underset{(l)}{-1}, \ldots\Big) \in \mathbb{R}^n, \Gamma_{ij}^{kl} > 0, \tag{7}$$

for any combination of indices $(i,j;k,l)$ such that $\Gamma_{ij}^{kl} > 0$ (dots stand for zeros). The conservation law (6) can be rewritten as $\mathbf{\Psi} \cdot \boldsymbol{\theta}_{ij}^{kl} = 0$, $\Gamma_{ij}^{kl} > 0$, where

$$\mathbf{\Psi} = (\Psi(\mathbf{v}_1), \ldots, \Psi(\mathbf{v}_n)) \in \mathbb{R}^n. \tag{8}$$

The set of vectors of reactions (7) with $\Gamma_{ij}^{kl} > 0$ can be written, one vector-row under another one, in the form of a matrix Λ. We call such matrix Λ the matrix of reactions of the model and the corresponding set of vectors of reactions (7), the set of reactions of the model (denoted by $\widetilde{\Lambda}$). The rank of the matrix Λ cannot, by the construction of the DVM, exceed $(n-(d+2))$, since for $\mathbf{v} = (v^{(1)}, \ldots, v^{(d)})$, the functions

$$\Psi_0(\mathbf{v}) = 1;\ \Psi_\alpha(\mathbf{v}) = v^{(\alpha)}, \qquad \alpha = 1, \ldots, d;\ \Psi_{d+1}(\mathbf{v}) = |\mathbf{v}|^2 \tag{9}$$

lead to $(d+2)$ linearly independent vectors (8) of conservation laws.

Hence, the DVM is normal if and only if the rank $r(\Lambda) = n-(d+2)$, provided that the vectors (8), (9) are linearly independent. This idea helps to reject the "*bad*" (not normal) DVMs; however, it says nothing about the way to construct normal models.

Our goal is to describe and construct all distinct non-degenerate normal DVMs for elastic collisions $\{V, \Lambda(V)\}$, where V (2) is the velocity set and $\Lambda(V)$ represents the matrix of reaction of the model, when the order $n \geq 4$ and the dimension $d \geq 2$ are given. By "non-degeneracy" we mean the following.

Definition 2. The velocity set V of an elastic DVM is said to be non-degenerate *if the equalities $a + \mathbf{b} \cdot \mathbf{v}_k + c|\mathbf{v}_k|^2 = 0$, $\mathbf{b} \in \mathbb{R}^d$, $a, c \in \mathbb{R}$, $k = 1, \ldots, n$, imply $a = c = 0$, $\mathbf{b} = 0$. Otherwise the set is said to be* degenerate. *The same terminology is used for corresponding DVMs $\{V, \Lambda(V)\}$.*

It is clear that each normal non-degenerate DVM in $\mathbb{R}^d$ has $p = d+2$ basic linearly independent invariants: $\mathbf{u}_1(V) = (1, \ldots, 1)$, $\mathbf{u}_\alpha(V) = (v_1^{(\alpha-1)}, \ldots, v_n^{(\alpha-1)})$ where $\alpha = 2, \ldots, d+1$ and $\mathbf{u}_{d+2}(V) = (|\mathbf{v}_1|^2, \ldots, |\mathbf{v}_n|^2)$, corresponding to the $p = d+2$ conservation laws for the spatially homogeneous version of eq. (9)

$$\sum_{k=1}^n f_k(t) = \text{const} \in \mathbb{R}_+; \quad \sum_{k=1}^n f_k(t)\mathbf{v}_k = \text{const} \in \mathbb{R}^d; \quad \sum_{k=1}^n f_k(t)|\mathbf{v}_k|^2 = \text{const} \in \mathbb{R}_+. \tag{10}$$

Following [10, 11], we introduce the space of invariants $U(V) = \operatorname{Span}\{\mathbf{u}_\alpha(V), \alpha = 1, \ldots, d+2\}$, and the space of reactions $L(V) = \operatorname{Span}\{\widetilde{\Lambda}(V)\}$, where $\widetilde{\Lambda}(V)$ is the set of reactions of the model. Then, for any non-degenerate normal DVM, we obtain $L \oplus U = \mathbb{R}^n$, $\dim U = d+2$, $\dim L = n-d-2$, where $\oplus$ denotes the orthogonal sum. The set $\widetilde{\Lambda}(V)$ contains at most $(n-d-2)$ linearly independent vectors of reactions, which can be chosen, generally speaking, in a non-unique way. We shall see below that any collection of such vectors is sufficient to find the velocity set V, though there are some special cases when this problem has several non-trivial solutions. Thus, we can characterise any normal non-degenerate d-dimensional DVM by a "basic" set $\widetilde{\Lambda}'$ of $(n-d-2)$ linearly independent reactions, omitting all their linear combinations. The corresponding $(n-d-2) \times n$ matrix Λ', whose rows are the vectors of reactions, will be considered as the matrix of reactions of the model. Primes are omitted below. The main idea behind the description of all normal non-degenerate DVMs in $\mathbb{R}^d$, with n velocities, is very simple.

Any such model has exactly $(n-d-2)$ linearly independent vectors of reactions. These vectors form a matrix with $(n-d-2)$ rows and n columns. Each row has only four non-zero elements, two ones and two minus ones (7). It is obvious that the total number $N(d,n)$ of such matrices (with a given pair of numbers $d \geq 2$ and $n \geq d+2$) is finite. Moreover, this number can be significantly reduced if we note that all matrices obtained by permutations of columns or rows correspond to the same model. The most general method is to generate all such matrices by computer and then to decide, by using some algorithm (see sect. **3**), whether or not the given matrix is a matrix of reactions of some "real" DVM. Each DVM is completely defined by its velocity set V, since all possible elastic collisions are allowed. This motivates the following definition.

Definition 3. Two DVMs with the velocity sets $V = \{\mathbf{v}_1, \ldots, \mathbf{v}_n\} \subset \mathbb{R}^d$ *and* $V' = \{\mathbf{v}'_1, \ldots, \mathbf{v}'_n\} \subset \mathbb{R}^d$ *are said to be* equivalent *if* V' *can be obtained from* V *by a sequence of the following operations: a) change of numeration of velocities; b) rotations, reflections and translations in* $\mathbb{R}^d$*; c) scaling transformations* $\mathbf{v}'_i = \alpha \mathbf{v}_i$ *in* $\mathbb{R}^d$.

Our aim is to construct all distinct (non-equivalent) normal DVMs. The first step is to reduce the number of possible sets $\widetilde{\Lambda}$ of reactions by demanding that the model should have exactly n distinct velocities.

Definition 4. The set $\widetilde{\Lambda}$ *of* m *linearly independent vectors is said to be* admissible *if* $\mathbf{e}_k - \mathbf{e}_l \notin \operatorname{Span} \widetilde{\Lambda}$*,* $1 \leq k < l \leq n$*, for any pair of unit vectors in* $\mathbb{R}^n$*. A matrix* Λ *of reactions is said to be* admissible *if the corresponding set of reactions* $\widetilde{\Lambda}$ *is admissible.*

Lemma 1. The condition $\mathbf{v}_k \neq \mathbf{v}_l$ *for* $k \neq l$ *is fulfilled for all* $\mathbf{v}_i \in V$ *(2),* $i = 1, \ldots, n$*, if and only if the corresponding set* $\widetilde{\Lambda}$ *of reactions of the normal model is admissible.*

Any DVM with n distinct velocities has an admissible set of reactions $\widetilde{\Lambda}$. This leads to certain restrictions on the set of possible matrices Λ for normal DVMs. In the plane case $d = 2$, all normal models with $n \in \{7, 8\}$ velocities can be obtained from two 6-velocity models by 1-extentions. This is not true, however, for $n \geq 9$, where we find "irreducible" normal models (that can not be obtained by 1-extension of some normal model).

3. – General algorithm for the construction of normal DVMs

We consider a $(n-d-2) \times n$ matrix Λ with $(n-d-2)$ linearly independent rows of the form (7) and assume that Λ is a matrix of reactions of a non-degenerate DVM $\{V, \Lambda(V)\}$. How to find the velocity set $V = \{\mathbf{v}_1, \ldots \mathbf{v}_n\} \subset \mathbb{R}^d$? Of course, such set is not unique since rotations, reflections, translations and scaling transformations of velocities do not change the matrix Λ. Our goal is to find at least one appropriate set V. We note that we can always use a permutation of columns of Λ together with a corresponding change of velocities. On the other hand, any matrix Λ has a rank $r(\Lambda) = n-d-2$, and can be transformed by permutation of columns to the form

$$\Lambda = \left(\begin{array}{c|c} B_{(n-p)\times p} & A_{(n-p)\times(n-p)} \end{array} \right). \tag{11}$$

Note that the matrix B contains $p = d+2$ columns which correspond to a subset of velocities $V_1 = \{\mathbf{v}_1, \ldots, \mathbf{v}_p\}$. The following statement explains in terms of V_1 when the above representation is valid.

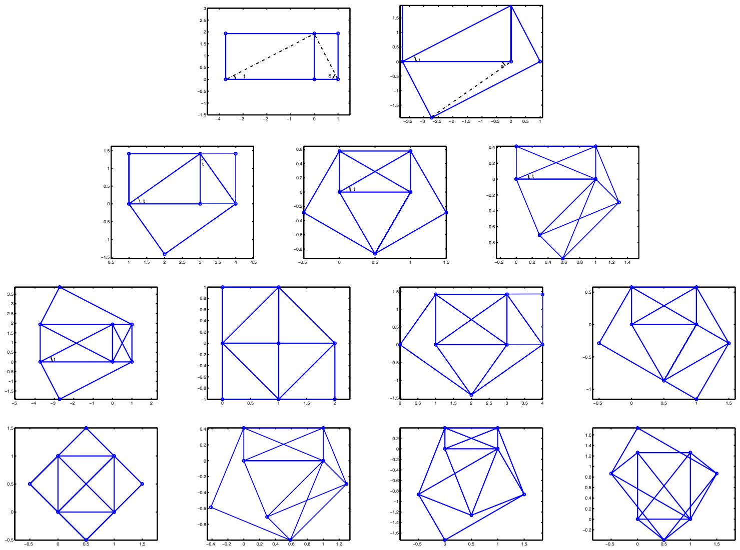

Fig. 1. – All normal DVMs with up to 8 velocities.

Lemma 2. Let Λ *be a* $(n-p)\times n$ *matrix of a non-degenerate DVM. Then the condition* $\det A \neq 0$ *in the representation* (11) *of* Λ *is valid if and only if the corresponding subset* $V_1 \subset V$ *is non-degenerate (see Definition 2).*

One can apply Lemma 2 to our problem of finding the velocity set $V = \{\mathbf{v}_1, \ldots, \mathbf{v}_n\}$ for a given matrix Λ. The method is presented in [12]. We present below the steps of the general algorithm for the construction of normal elastic DVMs in any dimension and for any number of velocities.

Step 1. Generate all $(n-d-2)\times n$ Λ-matrices having as rows $(n-d-2)$ linearly independent vectors of type (7). In addition, these matrices should be admissible. The set $\Theta = \{\Lambda_1, \ldots, \Lambda_N\}$, of all generated matrices Λ, is obviously finite.

Step 2. For $j = 1, \ldots, N$ take $\Lambda = \Lambda_j \in \Theta$. Suppose that there exists a normal discrete DVM with the matrix Λ of reactions and denote by $\mathbf{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_n), \mathbf{x}_k \subseteq \mathbb{R}^d$, $k = 1, \ldots, n$, the vector of velocities of the model. Denote $\widetilde{\mathbf{X}} = (|\mathbf{x}_1|^2, \ldots, |\mathbf{x}_n|^2)$. Check the solvability of the system

$$
(12) \qquad \begin{cases} \Lambda \mathbf{X} = \mathcal{O}_{(n-d-2)\times d}, \\ \Lambda \widetilde{\mathbf{X}} = \mathcal{O}_{(n-d-2)\times 1}, \end{cases}
$$

where $\mathcal{O}_{i\times j}$ is the $(i \times j)$ null-matrix. A general way to check the solvability of the system (12) is discussed in [12]. The case of small number of velocities $n \le 10$ is discussed below.

4. – Normal plane elastic models with $n \le 8$ velocities

From the geometrical point of view, a normal plane elastic model is a lattice of rectangles. The simplest model has six vertices (velocities) and two independent rectangles; for normal models, the number p of independent rectangles is given by the equality

$p = n - d - 2$, where n is the number of points and d is the dimension. All 6-velocity normal models contain two independent rectangles having two vertices in common. Hence, they contain: (a) two rectangles that share one side; (b) two rectangles having a diagonal in the first rectangle as a side in the second one; (c) two rectangles that share one diagonal. The last case represents a degenerate model. The two normal 6-velocity models are illustrated in fig. 1 (first row) and their corresponding Λ -matrices are

$$\Lambda_{(a)} = \begin{pmatrix} 1 & -1 & 1 & -1 & 0 & 0 \\ 1 & 0 & 0 & -1 & 1 & -1 \end{pmatrix}, \qquad \Lambda_{(b)} = \begin{pmatrix} 1 & -1 & 1 & -1 & 0 & 0 \\ 1 & 0 & -1 & 0 & 1 & -1 \end{pmatrix}. \tag{13}$$

Using the 1-extension method [7], we construct all distinct normal models [10] for $n \leq 8$: three 7-velocity normal models (fig. 1, second row) and eight 8-velocity normal models (fig. 1, last two rows). All normal models with $n \leq 8$ are reducible [10], *i.e.* are 1-extensions [7]. This is however not true for $n \geq 9$ as we shall see below.

5. – Algorithm for the construction of normal plane elastic models with small number of velocities

One can prove [10] that all normal models of order $n \leq 10$ contain a 6-velocity normal model (fig. 1). Because of the invariance under rotations, reflections, translations and scaling transformations, the first components of the vector X of phase points of the model are: $\mathbf{x}_1 = (0,0)$; $\mathbf{x}_2 = (1,0)$; $\mathbf{x}_3 = (1,\theta)$; $\mathbf{x}_4 = (0,\theta)$, $\theta \in \mathbb{R}_+$. Hence, we can partition the normal models in two classes: i) models that contain a 6-velocity normal model of type (a); ii) models that contain a 6-velocity normal model of type (b).

The system (12) can be then rewritten in the case i) as

$$\begin{cases} \mathbf{x}_1 = (0,0);\ \mathbf{x}_2 = (1,0);\ \mathbf{x}_3 = (1,\theta);\ \mathbf{x}_4 = (0,\theta),\ \theta \in \mathbb{R}_+, \\ \mathbf{x}_5 = (\mu,\theta);\ \mathbf{x}_6 = (\mu,0),\ \mu \in \mathbb{R}\backslash\{0,1\}, \\ \mathbf{x}_k = (a_k^{'}, b_k^{'}),\ k = 7,\dots,n, \\ \Lambda X = 0,\ X = (\mathbf{x}_1,\dots,\mathbf{x}_n),\ \mathbf{x}_k \in \mathbb{R}^2,\ k = 1,\dots,n, \\ \Lambda \widetilde{X} = 0,\ \widetilde{X} = (|\mathbf{x}_1|^2,\dots,|\mathbf{x}_n|^2) \end{cases} \tag{14}$$

and in the case ii), as the system (14) with modified $\mathbf{x}_5 = (1-\mu\theta, \theta+\mu)$, $\mathbf{x}_6 = (-\mu\theta, \mu)$, $\mu \in \mathbb{R}\backslash\{0\}$. Since for $n \leq 10$ all normal models have a corresponding Λ-matrix of reactions which contains a 6-velocity model of type (a) or type (b), and since interchanging rows or columns lead to equivalent models, we can state that all matrices corresponding to normal models of order n can be expressed as

$$\Lambda = \left(\begin{array}{c|c} \Lambda_{(a),(b)} & O_{2\times(n-6)} \\ \hline B^{'}_{(n-6)\times 6} & A^{'}_{(n-6)\times(n-6)} \end{array} \right), \tag{15}$$

where $\Lambda_{(a),(b)}$ is one of the matrices $\Lambda_{(a)}$ or $\Lambda_{(b)}$ in (13). Using Lemma 2 one can prove that the matrix $A^{'}$ in (15) is invertible, *i.e.* $\det A^{'} \neq 0$. The following algorithm contains the same two steps as in the general case described in sect. **3**.

Step 1A. Generate all admissible matrices Λ_j, $j = 1 \dots N$, for reducible models. To find reducible models (1-extensions), only one new velocity is added to an already existing

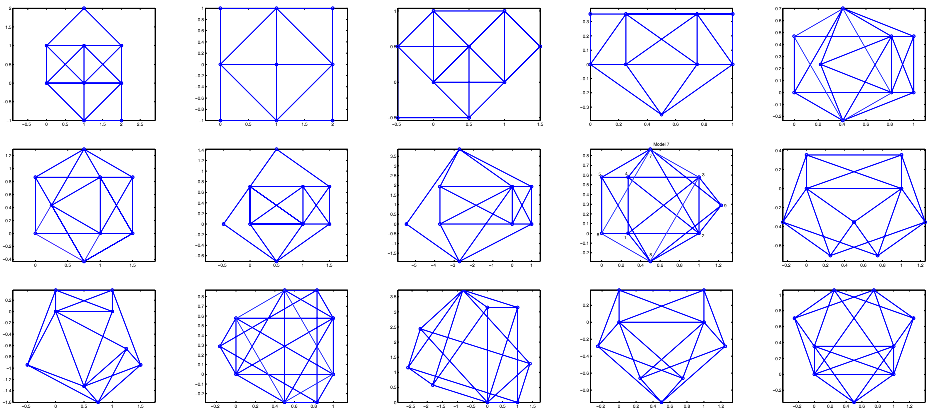

Fig. 2. – All 9-velocity normal DVMs.

$(n-1)$-velocity normal model, *i.e.* to a given $(n-1)\times(n-5)$ matrix, corresponding to an $(n-1)$-velocity normal model, we need to add one new column containing only zeros, and then add one new row of length n. The last element in the new row must be either 1 or (-1). The rest of the row must be created in the way that, in total, it contains two 1 and two (-1), and the remaining elements are 0. We generate all possible rows and add them to all $(n-1)$-velocity models and get us all Λ_j matrices for 1-extensions, with $N = 105$ for $n = 8$, $N = 784$ for $n = 9$, and $N = 2520$ for $n = 10$. Continue to step 2.

Step 1B. Generate all admissible matrices Λ_j, $j = 1 \dots N$, for irreducible models. We divide all possible matrices in two cases, Case i) with Λ_a and Case ii) with Λ_b, as the first two rows filled with zeros in the $(n-6)$ remaining columns. Then we generate all possible outcomes of the remaining $(n-6)$ rows, where the following properties must be fulfilled: a) each row must contain two (-1), two 1, and the rest 0; b) in two different rows, one cannot have three nonzeros in common (since three vertices define completely a rectangle); c) multiplying one row with (-1), makes no difference; d) interchanging rows gives equivalent models; e) the matrix must be admissible (the model must have exactly n distinct velocities (Lemma 1)): to check this, one row containing one element

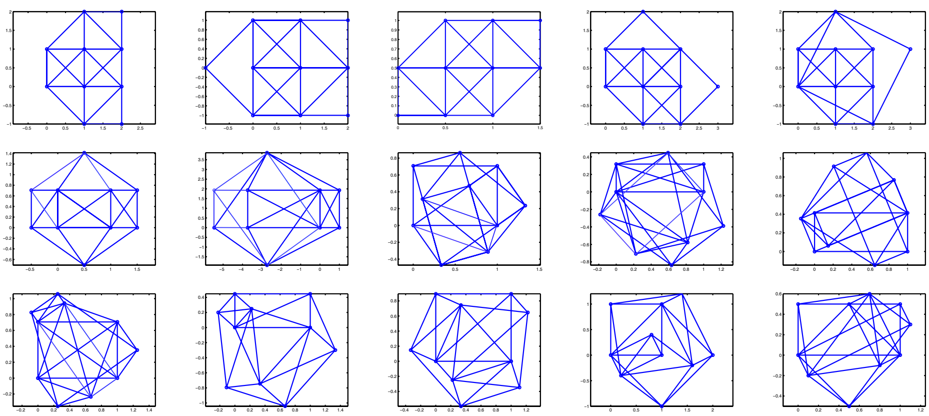

Fig. 3. – All 10-velocity normal DVMs.

1, one element (-1), and the rest zero, is added to the $n \times (n-4)$-matrix; the new $n \times (n-3)$-matrix should have a rank equal to $(n-3)$; f) in all columns we should have at least two non-zeros (only one non-zero corresponds to possible matrices for 1-extension models, already taken care of in Step 1A); g) $\det \Lambda(3:n-4, 7:n) \neq 0$.

For $n = 8$ we obtain no matrices satisfying the conditions a)-g) (*i.e.* all 8-velocity normal DVMs are 1-extensions). For $n = 9$ we get $N = 7779$ matrices (3486 from Case i) and 4293 from Case ii)), and for $n = 10$ the number of matrices is $N = 7515893$ (3416565 from Case i) and 4099328 from Case ii)).

Step 2. Verify the solvability of the system (14), *i.e.* verify if a given matrix Λ_j gives a normal n-velocity model. If the system has a solution (or solutions), a normal n-velocity model(s) is found. Step 2 is repeated until all Λ_j are checked.

By implementing the above given algorithm we get the complete result for the cases $n \in \{9, 10\}$: nine 9-velocity normal DVMs that are 1-extensions (first nine models in fig. 2), six 9-velocity normal DVMs that are not 1-extensions (last six models in fig. 2), nine 10-velocity normal DVMs that are 1-extensions (first nine models in fig. 3), six 10-velocity normal DVMs that are not 1-extensions (last six models in fig. 3).

6. – Conclusions

The main result of this paper is the complete classification (description of all different models) of plane normal DVMs with small number of velocities (up to 10). All models with up to 8 velocities are reducible (results of the 1-extensions method [6]). For $n \geq 9$ we also find irreducible normal models. Our algorithm allows us to give a full description of all possible non-equivalent normal DVMs in any dimension and with any number of velocities. We hope to consider the related $3d$ problems in the future publication.

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