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LETTER TO THE EDITOR

A triangularization algorithm which determines the Lie symmetry algebra of any system of PDEs

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Abstract. We present several algorithms which have been automated in the symbolic language MACSYMA. Algorithm STANDARD FORM reduces any system of linear PDEs to a simplified triangular form which has its integrability conditions identically satisfied. Generally a system's standard form is more amenable to numerical or analytical solution techniques than the system itself. The dimension of the solution space and the consistency or inconsistency of a system are directly determinable from its standard form. Algorithm TAYLOR uses a system's standard form to compute its Taylor series solution to any prescribed finite degree. We present an algorithm STRUCTURE CONSTANT based on STANDARD FORM and TAYLOR which, unlike existing symbolic algorithms for determining symmetries, *always* computes the dimension and structure constants of the Lie symmetry algebra of any system of PDEs.

Systems of linear algebraic equations which arise in applications seldom appear in simplest form. However such systems can be converted to row-reduced echelon form by applying a finite number of elementary row operations. This triangularized form expresses certain (leading) variables as linear combinations of other (parametric) variables which can be assigned arbitrary values. The dimension of the solution space of a system is equal to the number of its parametric variables.

We present an algorithm (STANDARD FORM) which brings arbitrary systems of linear PDEs in m independent variables $x=(x_1, x_2, \ldots, x_m)$ and n dependent variables $V=(V_1(x), \ldots, V_n(x))$ to a simplified triangular form by applying a finite number of elementary operations consisting of additions, multiplications and differentiations. The standard form has all of its integrability conditions satisfied and is based on the classical theory of involutive systems [1, 2] (see [9] for a REDUCE program for constructing involution systems). If two systems of PDEs in the same dependent and independent variables have the same general solution then their standard forms are identical. The standard form of a system expresses certain leading derivatives of the V_p as functions of other parametric derivatives. All derivatives of the V_p that cannot be obtained by differentiation of leading derivatives of the standard form are called parametric derivatives. The algorithm which determines this parametric set is called INITIAL DATA since the assignment of values to the parametric derivatives at an initial point $x=x^0$ uniquely determines the values of all other derivatives of the V_p at $x=x^0$. The dimension of the solution space of a system is equal to the number of parametric derivatives and may be finite or infinite. Algorithm TAYLOR uses a system's standard form and initial data to compute its Taylor series solution about a point $x=x^0$ to any desired finite degree.

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We consider the application of the above algorithms to the associated overdetermined systems of linear homogeneous PDEs (the determining equations) whose solution determines the infinitesimal generators of the Lie symmetry algebra of a given system of PDEs. The physical importance of finding symmetries of PDEs [3, 4] has led to the development of heuristic-based symbolic programs for setting up and attempting to solve determining equations [5, 6]. A heuristic-free algorithm STRUCTURE CONSTANT is presented which determines both the dimension and structure constants of the Lie symmetry algebra of any system of PDEs in a finite number of steps. Our work complements integration-dependent techniques [5, 6] in that the standard form of a determining system is often more amenable to explicit solution by these techniques than the original system. In [7] our methods are extended to form an algorithm that group classifies entire classes of PDEs depending on variable coefficients. For example when this method is applied to group classification of the nonlinear telegraph system

$$\phi_t = \psi_y \qquad \phi_y = C(\psi)\psi_t + B(\psi) \tag{1}$$

it reveals [7] that (1) has an infinite parameter Lie symmetry group if the variable coefficients B, C satisfy the classification conditions $C' = 2B'C/B$, $B'' = 2(B')^2/B$. In these cases (1) is exactly linearizable [3, 8] and $B(\psi) = \kappa_1/(\psi - \lambda)$, $C(\psi) = \kappa_2/(\psi - \lambda)^2$. In addition if $B(\psi) = \kappa_1\psi^{\nu_1}/[1 + \nu_3\psi^{\nu_1}]$ and $C(\psi) = \kappa_2\psi^{\nu_2}/[1 + \nu_3\psi^{\nu_1}]^2$ then system (1) possesses [7] a non-trivial Lie symmetry with generator

$$\underline{L} = [(2\nu_1 - \nu_2 - 2)y/2 - \nu_3\nu_1\phi/\kappa_1]\frac{\partial}{\partial y} + \left[(\nu_1 - \nu_2 - 1)t - \frac{\nu_3\nu_1}{\kappa_1}\int_0^{\psi} C(z)\,\mathrm{d}z\right]$$
$$- \psi\frac{\partial}{\partial\psi} - \tfrac{1}{2}(2 + \nu_2)\phi\frac{\partial}{\partial\phi}.$$

The constants $\kappa_1, \kappa_2, \nu_1, \nu_2, \nu_3, \lambda$ are arbitrary and can be used as fitting parameters in physical applications.

The derivatives of the V_p (including zeroth-order derivatives) will be denoted by $\partial^{a_1+\ldots+a_m}V_p/\partial x_1^{a_1}\ldots\partial x_m^{a_m} := D_aV_p$ where $a = (a_1, \ldots, a_m)$ and $\mathrm{ord}(a) := a_1 + \ldots + a_m \geqslant 0$ is called the order of the derivative. We define the following total ordering $>_s$ on the set of derivatives (other orderings are possible [2]).

We say that $D_aV_p >_s D_bV_q$ if (i) $\mathrm{ord}(a) >_x \mathrm{ord}(b)$, or, (ii) $\mathrm{ord}(a) = \mathrm{ord}(b)$ and $p < q$, or, (iii) $\mathrm{ord}(a) = \mathrm{ord}(b)$, $p = q$ and $a >_{\mathrm{lex}} b$, where the lexicographical ordering $>_{\mathrm{lex}}$ is defined by $a >_{\mathrm{lex}} b$ iff the first non-zero $a_k - b_k > 0$.

The *leading derivative* for an equation is the unique derivative in the equation which is highest in the ordering $>_s$.

Algorithm 1: STANDARD FORM ($\boldsymbol{\Phi}$)

Input: Any system of linear PDEs $\boldsymbol{D}$ with dependent variables $V_1, V_2, \ldots, V_n$ and independent variables $x_1, \ldots, x_m$.

Output: If $\boldsymbol{D}$ is consistent then STANDARD FORM returns a system of linear PDEs $\boldsymbol{\Phi}(\boldsymbol{D})$ having the same solution as $\boldsymbol{D}$ in the solved form

$$D_bV_p = f_{pb} \tag{2}$$

where $D_bV_p \in \mathscr{L}$ and

(i) the derivative on the LHS of any equation in (2) is strictly higher in the ordering

$>_s$ than any derivative in the RHS of the same equation (we call $\mathscr{L}$ the set of leading derivatives for (2));

(ii) no derivative appears on both the LHS and RHS of (2);

(iii) the derivatives on the LHS of (2) are all distinct;

(iv) no derivative in (2) is a non-trivial derivative of any derivative on the LHS of (2);

(v) the integrability conditions of (2) are identically satisfied modulo all lexicographic substitutions which follow from (2).

Method

1.0. Set $\hat{\boldsymbol{D}} = \boldsymbol{D}$.

1.1. From the set of equations in $\hat{\boldsymbol{D}}$ which are not in solved-form with respect to their leading derivatives (i.e. have form $0 = $ RHS), select an equation with leading derivative which is highest in the ordering $>_s$ and solve it for this derivative (i.e. the equation now has the form *leading derivative* = RHS). Use the equation to eliminate all explicit occurrences of this leading derivative in the remaining equations of $\hat{\boldsymbol{D}}$. Repeat this process until $\hat{\boldsymbol{D}}$ is obtained in the form of a system which satisfies conditions (i), (ii) and (iii) above.

1.2. If any derivative in $\hat{\boldsymbol{D}}$ is a non-trivial derivative of any derivative on the LHS of $\hat{\boldsymbol{D}}$ then make the implicit substitution of the latter derivative into the former (if the derivative in which the substitution is made is a leading derivative then the equation to which it belongs is reverted to the form $0 = $ RHS). Continue this process until no further substitutions are possible.

1.3. If $\hat{\boldsymbol{D}}$ no longer satisfies conditions (i), (ii), (iii) then return to step 1.1; otherwise continue to step 1.4 with a system which now satisfies (i)–(iv).

1.4. Calculate the minimal integrability conditions $\boldsymbol{I}_{\min}$ of $\hat{\boldsymbol{D}}$. If $\boldsymbol{I}_{\min} \neq \varnothing$ when simplified modulo all lexicographic substitutions which follow from $\hat{\boldsymbol{D}}$ then append the simplified $\boldsymbol{I}_{\min}$ to $\hat{\boldsymbol{D}}$ and return to step 1.1. If $\boldsymbol{I}_{\min} = \varnothing$ then calculate the maximal integrability conditions $\boldsymbol{I}_{\max}$ and simplify these conditions subject to all lexicographic substitutions which follow from $\hat{\boldsymbol{D}}$. If $\boldsymbol{I}_{\max} = \varnothing$ then STANDARD FORM has terminated with a system $\boldsymbol{\Phi}(\boldsymbol{D}) = \hat{\boldsymbol{D}}$ satisfying conditions (i)–(v) above; if not $\boldsymbol{I}_{\max}$ is appended to $\hat{\boldsymbol{D}}$ and the system is returned to step 1.1.

If at any stage the algorithm uncovers a non-trivial equation of the form $0 = f(x)$ then the system is inconsistent and the algorithm returns that message.

We now define the terms lexicographic substitution, $\boldsymbol{I}_{\min}$, $\boldsymbol{I}_{\max}$ referred to in 1.4. Suppose $\hat{\boldsymbol{D}}$ is a system which satisfies conditions (i)–(iv) above. The unique substitution, if it exists, $D_a V_p = D_{a-b^*}(D_{b^*} V_p) = D_{a-b^*} f_{pb^*}$ where $D_{b^*} V_p$ is the leading derivative in $\mathscr{L}$ with greatest lexicographical index b^* such that $a_k \geqslant b_k{}^*$, $k = 1, \ldots, m$, is called a lexicographical substitution (thus for all $b \in \mathscr{L}$ with $b_k \geqslant a_k$, $b^* \geqslant_{\text{lex}} b$). When the total derivative $D_{a-b^*} F_{pb^*}$ has been evaluated, further lexicographic substitutions from $\hat{\boldsymbol{D}}$ may be possible. After a finite number of such substitutions, however, any derivative $D_a V_p$ is *uniquely* obtained as a function of *parametric derivatives only*, and we say that all possible lexicographic substitutions have been carried out.

For every distinct pair of equations $D_a V_p = f_{pa}$, $D_b V_p = f_{pb}$ in a system $\hat{\boldsymbol{D}}$ satisfying conditions (i)–(iv) it follows that for $c = (c_k)$ with $c_k \geqslant \max\{a_k, b_k\}$ we have the consistency conditions:

$$D_c V_p - D_c V_p = D_{c-a} f_{pa} - D_{c-b} f_{pb} = 0. \tag{3}$$

The *minimal integrability conditions* $\boldsymbol{I}_{\min}$ are the finite subset of the above conditions with $c_k = \max\{a_k, b_k\}$ such that there is no other condition of form (3) with $\hat{c} \neq c$ such that $\hat{c}_k \leq c_k$ for all k. The *maximal integrability conditions* $\boldsymbol{I}_{\max}$ are the finite subset of the conditions (3) where $\max\{a_k, b_k\} \leq c_k \leq \max_{D_{\bar{b}} V_p \in \mathscr{L}}\{\bar{b}_k\}$. Algorithm 1 eliminates equations in $\hat{\boldsymbol{D}}$ which are total derivatives of other equations in $\hat{\boldsymbol{D}}$, unlike the classical method for constructing involution systems [1, 2] which includes such equations. A smaller set of integrability conditions can be obtained through a more detailed construction involving our methods and those of [2].

Algorithm 2: INITIAL DATA
Input: The leading derivatives $\mathscr{L} = \{D_b V_p\}$ of a system $\boldsymbol{\Phi}(\boldsymbol{D})$ which is the standard form of a system $\boldsymbol{D}$.
Output: The parametric derivatives $\mathscr{P} = \{D_h V_p\}$ and $\dim(\boldsymbol{D})$ the dimension of the solution space of $\boldsymbol{D}$.
Method
2.1. $\mathscr{P} = \bigcup_{p=1}^{n} \mathscr{P}_p$ where $\mathscr{P}_p = \mathscr{W}_p(0) - \bigcup_{D_b V_p \in \mathscr{L}} \mathscr{W}_p(b)$ and $\mathscr{W}_p(a) = \{D_{c+a} V_p\colon\ c_k \geq 0, k = 1, \ldots, m\}$ is the set of derivatives obtainable from $D_a V_p$ by differentiation.
2.2. $\dim(\boldsymbol{D}) = \#(\mathscr{P})$ where $\#(\mathscr{P})$ is the number of elements in $\mathscr{P}$.

Although step 2.2 apparently requires the enumeration of infinite sets it is reducible to a finitely computable one by considering the intersection of these sets with the smallest boxes $\mathscr{B}_p(=\{D_a V_p\colon\ 0 \leq a_k \leq \max_{D_v V_p \in \mathscr{L}}\{b_k\}\})$ containing the leading derivatives of the V_p and the origin. In particular it is easily shown that $\mathscr{P}$ is finite iff for $p = 1, \ldots, n$ and $k = 1, \ldots, m$, $\exists D_b V_p \in \mathscr{L}$ with $b_l = 0$ for $l \neq k$ and then $\mathscr{P} = \bigcup_{p=1}^{n} \mathscr{B}_p \cap \mathscr{P}_p$; otherwise $\mathscr{P}$ is infinite and the initial data can be uniquely specified by a finite number of constants and arbitrary functions (see [1, 2, 7] and example 2).

Algorithm 3: TAYLOR (finite-dimensional case)
Input: The standard form $\boldsymbol{\Phi}(\boldsymbol{D})$ of a linear system $\boldsymbol{D}$, a fixed point x^0, a degree ζ and a set of initial data $D_h V_p|_{x=x^0} = \text{constant} = \alpha_s$ where $D_h V_p \in \mathscr{P}$ and the label s has been chosen so that $s = 1, 2, \ldots, \dim(\boldsymbol{D})$.
Output: Taylor series representation of the solution of $\boldsymbol{D}$ to degree ζ subject to the above initial data.
Method
3.1. For $\operatorname{ord}(a) \leq \zeta$ use repeated lexicographic substitutions from $\boldsymbol{\Phi}(\boldsymbol{D})$ to express $D_a V_p$, $p = 1, \ldots, n$, as a function of parametric derivatives only.
3.2. Evaluate $D_a V_p$ at $x = x^0$ to obtain $H^s_{pa}(x^0)$: $D_a V_p|_{x=x^0} = \Sigma_{s=0}^{\dim(\boldsymbol{D})} \alpha_s H^s_{pa}(x^0)$.
3.3. Form the Taylor series for $V_p(x)$ to degree ζ about $x = x^0$.
3.4. By substituting for $D_a V_p|_{x=x^0}$ from 3.2 into the Taylor series for $V_p(x)$ found in 3.3 obtain a series representation for a basis of solutions $V^s_p(x)$ for $\boldsymbol{D}$ to degree ζ

$$V^s_p(x) = \sum_{\operatorname{ord}(a) \leq \zeta} H^s_{pa}(x^0) \frac{(x_1 - x^0_1)^{a_1} \ldots (x_m - x^0_m)^{a_m}}{a_1! \ldots a_m!} + \mathcal{O}(\zeta + 1) \tag{4}$$

where $V_p(x) = \Sigma_{s=0}^{\dim(\boldsymbol{D})} \alpha_s V^s_p(x)$. If $\boldsymbol{D}$ is an inhomogeneous linear system then $s = 0$, $\alpha_0 = 1$ and $V^0_p(x)$ corresponds to the inhomogeneous term in the solution $V_p(x)$. In the homogeneous case $V^0_p(x) = 0 = H^0_{pa}(x^0)$.

If the coefficients in the f_{pb} in (2) are real analytic functions of x in some neighbourhood of x^0 then the above series converge uniformly and absolutely in some neighbourhood of x^0 [1, 2]. Algorithm TAYLOR can be easily extended to cover the infinite dimensional case.

Algorithm 4: STRUCTURE CONSTANT (finite-dimensional case)
Input: Standard form $\boldsymbol{\Phi}(\boldsymbol{D})$ of the determining equations $\boldsymbol{D}$ for the infinitesimals $(\xi_i(x), \eta_j(x)) = (V_p(x))$ characterizing the symmetries of a given system of PDEs $\boldsymbol{A}$; initial data and $\dim(\boldsymbol{D})$ as calculated by algorithm INITIAL DATA.
Output: The structure constants C^t_{rs} for the Lie symmetry algebra

$$[\underline{L}_r, \underline{L}_s] = \sum_{t=1}^{\dim(\boldsymbol{D})} C^t_{rs}\underline{L}_t \qquad 1 \leq r < s \leq \dim(\boldsymbol{D})$$

of the system of PDEs $\boldsymbol{A}$.
Method
4.1. Choose an initial value for the degree ζ.
4.2. Apply TAYLOR to $\boldsymbol{\Phi}(\boldsymbol{D})$ to obtain a series expansion about a fixed point $x = x^0$ to degree ζ for each member $V^l_k(x)$ of a basis for the infinitesimals $V_k(x)$.
4.3. Substitute the truncated series obtained in 4.2 into the commutation relations:

$$\sum_{k=1}^{m}\left[V^r_k(x)\frac{\partial V^s_l(x)}{\partial x_k} - V^s_k(x)\frac{\partial V^r_l(x)}{\partial x_k}\right] = \sum_{t=1}^{\dim(\boldsymbol{D})} C^t_{rs}V^t_l(x) \qquad l = 1, \ldots, m(=n). \tag{5}$$

4.4. Comparing powers in (5) and taking into account the order of remainder terms yields a finite number of linear equations for the C^t_{rs}. If these equations, when solved, completely specify the C^t_{rs} then the algorithm has terminated. Otherwise increase the degree to $\hat{\zeta} > \zeta$ and return to step 4.2.

Algorithm STRUCTURE CONSTANT terminates in a finite number of steps since its non-termination would imply the impossibility of needing an infinite number of linear equations to determine a finite number of unknowns (the C^t_{rs}). The method can be easily extended to identifying the structure and dimension of the maximal finite-dimensional subalgebra in the infinite-dimensional case [7]. STRUCTURE CONSTANT complements the results given in [10] which provide algorithms for classifying Lie algebras given that their structure constants are known.

Nonlinear systems $\boldsymbol{D}$ are also explicitly reducible to standard form provided that the nonlinear equations which arise can be explicitly solved for their leading derivatives. Choosing orderings other than the standard one $>_s$ can assist in this process. Even if an explicit reduction is not possible, judicious use of the implicit function theorem may still lead to partial results.

We conclude with examples illustrating the algorithms STANDARD FORM and INITIAL DATA.

Example 1. Consider $\boldsymbol{D} = \{0 = V_{2x_1x_1} - V_2,\ 0 = 2V_{1x_2x_2} + V_{1x_1x_1} - 2V_{2x_1} - V_2,\ 0 = V_{1x_1x_1x_2} - x_1V_2,\quad 0 = V_{2x_1} + V_{1x_1x_1} - 2V_2,\quad 0 = V_{1x_1x_2} - 3V_{2x_2} + (3x_1 - 1)V_2,\quad 0 = V_{2x_2} + V_{1x_1x_1} - (x_1+1)V_2,\ 0 = V_{1x_1x_1} - V_2\}$ where $V_r = V_r(x_1, x_2)$, $r = 1, 2$.
Step 1.1. $\hat{\boldsymbol{D}}$ consists of the equations: (a) $V_{1x_1x_1x_2} = x_1V_2$; (b) $V_{1x_1x_1} = V_2$; (c) $V_{1x_1x_2} = V_2$; (d) $V_{1x_2x_2} = V_2$; (e) $V_{2x_1x_1} = V_2$; (f) $V_{2x_1} = V_2$; (g) $V_{2x_2} = x_1V_2$.
Step 1.2. We have (a): $V_{1x_1x_1x_2} - x_1V_2 \overset{(b)}{=} V_{2x_2} - x_1V_2 \overset{(g)}{=} 0$ and (e): $V_{2x_1x_1} - V_2 \overset{(f)}{=} V_{2x_1} - V_2 \overset{(f)}{=} 0$. So equations (a) and (e) are removed from $\hat{\boldsymbol{D}}$.

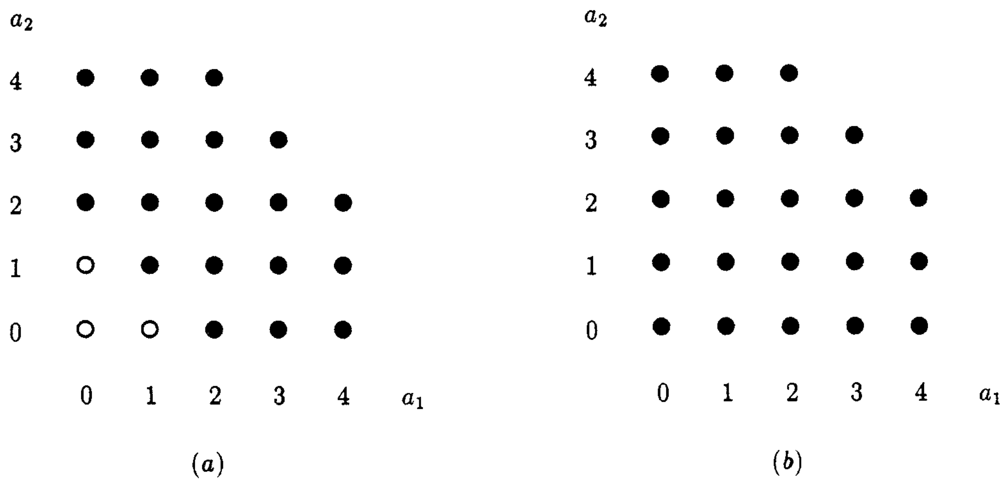

Figure 1. Graphical representation of the sets $\mathscr{P}_p$ of parametric derivatives for the systems in standard form arising from example 1. A ○ located at $(a_1,\ a_2)$ indicates that $\partial^{a_1+a_2}V_p/\partial x_1^{a_1}\partial x_2^{a_2}$ is a parametric derivative of V_p. (a) $p=1$, $V_{1x_1x_1}=V_{1x_1x_2}=V_{1x_2x_2}=0$. (b) $p=2$, $V_2=0$.

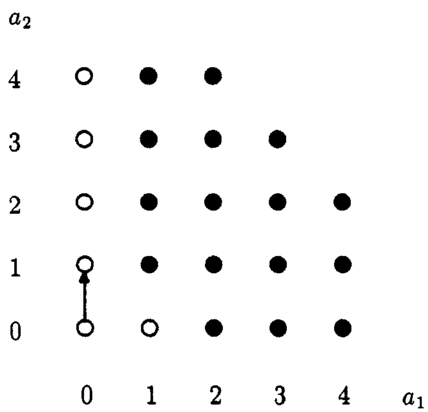

Figure 2. Same as figure 1, but for example 2. $p=1$, $V_{1x_1x_1}=V_{1x_1}$, $V_{1x_1x_2}=V_{1x_2}$.

Step 1.4. $\boldsymbol{I}_{\min}=\{0=V_{2x_2}-V_{2x_1},\ 0=V_{2x_1}-V_{2x_2},\ 0=V_{2x_2}-(V_2+x_1V_{2x_1})\}$. Simplification subject to lexicographic substitution from $\hat{\boldsymbol{D}}$ gives $\boldsymbol{I}_{\min}=\{0=(x_1-1)V_2,\ 0=(1-x_1)V_2,\ 0=-V_2\}\neq\emptyset$, so $I_{\min}$ is appended to $\hat{\boldsymbol{D}}$.
Step 1.1. We obtain $V_2=0$ and $\hat{\boldsymbol{D}}=\{V_{1x_1x_1}=0,\ V_{1x_1x_2}=0,\ V_{1x_2x_2}=0,\ V_2=0\}$. No change occurs at steps 1.2, 1.3. At step 1.4 $\boldsymbol{I}_{\min}=\boldsymbol{I}_{\max}=\emptyset$ so STANDARD FORM terminates with $\boldsymbol{\Phi}(\boldsymbol{D})=\hat{\boldsymbol{D}}$ above.
Step 2.1. $\dim(\boldsymbol{D})<\infty$ since $V_{1x_1x_1}$, $V_{1x_2x_2}$ and V_2 are in $\mathscr{L}$. So $\mathscr{P}=(\mathscr{B}_1\cap\mathscr{P}_1)\cup(\mathscr{B}_2\cap\mathscr{P}_2)=\{V_1,\ V_{1x_1},\ V_{1x_2}\}$.
Step 2.2. $\dim(\boldsymbol{D})=\#(\mathscr{P})=3$ (see figure 1) with corresponding initial data $V_1(x^0)=\alpha_1$, $V_{1x_1}(x^0)=\alpha_2$ and $V_{1x_2}(x^0)=\alpha_3$.

Example 2. Consider $\boldsymbol{D}=\{V_{1x_1x_1}=V_{1x_1},\ V_{1x_1x_2}=V_{1x_2}\}$ where $V_1=V_1(x_1,x_2)$ which is already in standard form. $\dim(\boldsymbol{D})=\infty$ since there is no equation of form $\partial^hV_1/\partial x_2^h=f$

in $\boldsymbol{D}$. $\mathscr{P} = \{D_{(1,0)}V_1\} \cup \{D_{(0,a_2)}V_1 : a_2 = 0, 1, 2, \ldots\}$. Equivalently the initial data and general solution of $\boldsymbol{D}$ depends on a single parameter $D_{(1,0)}V_1|_{x=x^0}$ and a single arbitrary function $V_1(x_1^0, x_2) = g(x_2)$ along the direction $(0, 1)$) (see figure 2 and for general treatments [2, 7]).

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