

Nonlinear Patterns in Chemical Networks as Symmetries of Transformation Groups

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Z. Naturforsch. **32a**, 1457–1464 [1977]; received July 9, 1977

The origin of a stable spatial pattern in chemical reaction systems has been traced back to symmetries characterized by one-parameter transformation groups. The chemical reaction-diffusion system of Dreitlein and Smoes served as a model for the mathematical approach. The procedure is based on the conversion of sets of partial differential equations to equivalent systems of first order in more parameters. The latter generally admit one-parameter groups, which are related to singularities observed as pattern. It is also shown how models may be constructed from Lie-algebras using the constraints of integrability.

Introduction

Pattern formation in nonlinear dynamic systems is a difficult subject to study. Not only are the mathematical descriptions cumbersome, if possible at all, but also the corresponding experiments sometimes display unexpected effects. In physics, a classical example of a pattern formation of this type is the array of hexagonal cells formed in the Benard [1] experiment. The hexagonal cell pattern in a liquid is maintained by a temperature gradient perpendicular to the surface. The hydrodynamic state of the circulating flow of the liquid within the cells may be described by a set of nonlinear partial differential equations. The same set also applies to pattern phenomena like turbulence in vortices [2] and to nonlinear waves. Similar difficulties are encountered in weather forecasting. These are only a few examples of patterns arising from nonlinear processes, which are found throughout the cosmos from its micro to its macro scale.

In the present paper, pattern formation in chemical reaction systems is treated. The basic procedure used is an extension of the methods developed in a previous article [3]. Firstly, the reaction-diffusion equation proposed by Dreitlein and Smoes [4] is considered as an example. The solutions of the system of partial differential equations are considered as a continuous multi-parameter group, the elements of which are represented by Lie series. This concept allows the recast of the set of partial differential equations in a system of nonlinear differential equations of first order in

more than one parameter. Subsequently, one-parameter transformation groups of the system can be found, which leave the latter system invariant. These groups are related to singular solutions, as already pointed out in the previous paper [3]. The relation of the spatio-temporal pattern to singular solutions is derived from the chemical model. The generalization of these results demonstrates the importance of Lie-algebras and the integrability conditions in this endeavour.

Mathematical details of transformation groups [5] and vector spaces [6] are presented elsewhere and will not be reviewed here. Finally, the notation of vector spaces is used to summarize the conditions derived for singularities in equations of forms.

The Reaction-Diffusion Model

The kinetics and spatio-temporal distribution of a two-variable model has been studied by Dreitlein and Smoes [4]. The nonlinear partial differential equations of the system are given in their dimensionless form by [7]:

$$\begin{aligned} \frac{\partial}{\partial t} a_1 - D_1 \frac{\partial^2}{\partial x^2} a_1 &= (E - a_1^2 - a_2^2) a_1 \\ &+ S a_2 - 2 R a_1 = F_1, \\ \frac{\partial}{\partial t} a_2 - D_2 \frac{\partial^2}{\partial x^2} a_2 &= (E - a_1^2 - a_2^2) a_2 \\ &- S a_1 + 2 R a_2 = F_2, \end{aligned} \quad (1)$$

where the dependent variables a_1 , a_2 are species quantities (component densities). The parameters D_1 , D_2 , E , S , and R are real constants and t , x are independent variables corresponding to time and space, respectively.

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In the following, the right hand side of Eqs. (1) is abbreviated as F_1 and F_2 respectively.

Equations (1) are equivalent to the following system of differential equations of first order in two independent variables (t, x):

$$\begin{aligned} \frac{\partial}{\partial t} a_1 &= a_3, & \frac{\partial}{\partial t} a_2 &= a_4, \\ \frac{\partial}{\partial x} a_1 &= a_5, & \frac{\partial}{\partial x} a_2 &= a_6, \\ \frac{\partial}{\partial x} a_5 &= \frac{1}{D_1} (a_3 - F_1), \\ \frac{\partial}{\partial x} a_6 &= \frac{1}{D_2} (a_4 - F_2), \end{aligned} \quad (2a)$$

where a_i ($i = 3, 4, 5, 6$) are defined by the upper four equations.

Equations (2a) may be complemented by the equations:

$$\begin{aligned} \frac{\partial}{\partial t} a_3 &= g_1, & \frac{\partial}{\partial t} a_4 &= g_2, & \frac{\partial}{\partial t} a_5 &= g_3, \\ \frac{\partial}{\partial t} a_6 &= g_4, & \frac{\partial}{\partial x} a_3 &= g_5, & \frac{\partial}{\partial x} a_4 &= g_6, \end{aligned} \quad (2b)$$

where the functions g_i ($i = 1, \dots, 6$) satisfy the integrability conditions

$$\begin{aligned} \partial^2 a_1 / \partial x \partial t &= \partial^2 a_1 / \partial t \partial x; \\ \partial^2 a_2 / \partial x \partial t &= \partial^2 a_2 / \partial t \partial x \quad \text{etc.} \end{aligned}$$

It follows that:

$$\begin{aligned} g_5 &= g_3; \quad g_6 = g_4; \quad \frac{\partial}{\partial x} g_1 = \frac{\partial}{\partial t} g_3; \\ \frac{\partial}{\partial x} g_2 &= \frac{\partial}{\partial t} g_4, \\ \frac{\partial}{\partial x} g_3 &= \frac{\partial}{\partial t} \left\{ \frac{1}{D_1} (a_3 - F_1) \right\} = \frac{1}{D_1} \left\{ -\frac{\partial F_1}{\partial t} + g_1 \right\}, \\ \frac{\partial}{\partial x} g_4 &= \frac{\partial}{\partial t} \left\{ \frac{1}{D_2} (a_4 - F_2) \right\} = \frac{1}{D_2} \left\{ -\frac{\partial F_2}{\partial t} + g_2 \right\}. \end{aligned} \quad (3)$$

Thus, we have four equations for the four unknown functions: g_i ($i = 1, 2, 3, 4$).

Solutions of the system (2) of differential equations may be interpreted as transformations of initial points $a^0 = \{a_1^0, a_2^0, a_3^0, a_4^0, a_5^0, a_6^0\}$ into final points $a = \{a_1, a_2, a_3, a_4, a_5, a_6\}$ belonging to a parameter set (x, t). Such a transformation can be carried out by two infinitesimal generators, A_x, A_t , associated to x and t , respectively. The finite

transformation is then given by a multi-dimensional Lie-series:

$$a_i(x, t, a^0) = \sum_{r=0}^{\infty} \frac{1}{r!} (t A_t + x A_x)^r a_i|_{a=a^0}, \quad (4)$$

where a_i is a variable element of a .

The system of differential equations of first order in the independent variables (x, t) generated by the Lie series (4) is [8]:

$$\frac{\partial a_i}{\partial t} = \xi_i; \quad \frac{\partial a_i}{\partial x} = \eta_i, \quad (5a)$$

where the functions ξ_i, η_i depend on a_i .

The associated infinitesimal generators are:

$$A_t = \sum_{i=1}^6 \xi_i \frac{\partial}{\partial a_i}; \quad A_x = \sum_{i=1}^6 \eta_i \frac{\partial}{\partial a_i}. \quad (5b)$$

Comparison of Eq. (5a) with Eqs. (2) gives the generators (5b) by combining the equations with $\partial/\partial t$ and $\partial/\partial x$, respectively:

$$\begin{aligned} A_t &= a_3 \frac{\partial}{\partial a_1} + a_4 \frac{\partial}{\partial a_2} + g_1 \frac{\partial}{\partial a_3} + g_2 \frac{\partial}{\partial a_4} \\ &\quad + g_3 \frac{\partial}{\partial a_5} + g_4 \frac{\partial}{\partial a_6}, \\ A_x &= a_5 \frac{\partial}{\partial a_1} + a_6 \frac{\partial}{\partial a_2} + g_5 \frac{\partial}{\partial a_3} + g_6 \frac{\partial}{\partial a_4} \\ &\quad + \frac{1}{D_1} (a_3 - F_1) \frac{\partial}{\partial a_5} + \frac{1}{D_2} (a_4 - F_2) \frac{\partial}{\partial a_6}. \end{aligned} \quad (6)$$

The integrability condition for the system (5a, b) requires that the commutator of the generators A_t and A_x satisfies [8]:

$$[A_t, A_x] = 0. \quad (7)$$

Equation (7) ensures that x and t define a surface on which one reaches the same point by proceeding first along x and then along t as when one follows first t and then x . An explicit calculation of Eq. (7) leads to an equivalent set of Eqs. (3), which are:

$$g_5 = g_3, \quad g_6 = g_4, \quad (8a)$$

$$A_t g_3 = A_x g_1, \quad A_t g_4 = A_x g_2, \quad (8b)$$

$$A_x g_3 = -\frac{1}{D_1} \left\{ a_3 \frac{\partial F_1}{\partial a_1} + a_4 \frac{\partial F_1}{\partial a_2} - g_1 \right\}, \quad (8c)$$

$$A_x g_4 = -\frac{1}{D_2} \left\{ a_3 \frac{\partial F_2}{\partial a_1} + a_4 \frac{\partial F_2}{\partial a_2} - g_2 \right\}. \quad (8d)$$

If the Eqs. (8c, d) are solved with respect to the functions g_1 and g_2 , one obtains the following Eqs. (8b) in g_3 and g_4 :

$$\begin{aligned} a_3 \frac{\partial g_3}{\partial a_1} + a_4 \frac{\partial g_3}{\partial a_2} + (F_1' + D_1 A_x g_3) \frac{\partial g_3}{\partial a_3} + (F_2' + D_2 A_x g_4) \frac{\partial g_3}{\partial a_4} + g_3 \frac{\partial g_3}{\partial a_5} + g_4 \frac{\partial g_3}{\partial a_6} \\ = A_x F_1' + D_1 A_x^2 g_3, \quad (9) \\ a_3 \frac{\partial g_4}{\partial a_1} + a_4 \frac{\partial g_4}{\partial a_2} + (F_1' + D_1 A_x g_3) \frac{\partial g_4}{\partial a_3} + (F_2' + D_2 A_x g_4) \frac{\partial g_4}{\partial a_4} + g_3 \frac{\partial g_4}{\partial a_5} + g_4 \frac{\partial g_4}{\partial a_6} \\ = A_x F_2' + D_2 A_x^2 g_4, \end{aligned}$$

where

$$F_1' = a_3 \frac{\partial F_1}{\partial a_1} + a_4 \frac{\partial F_1}{\partial a_2} \quad \text{and} \quad F_2' = a_3 \frac{\partial F_2}{\partial a_1} + a_4 \frac{\partial F_2}{\partial a_2}.$$

The Eqs. (9) are nonlinear in the derivatives and hence are still more complicated than the Equations (1).

When the Eqs. (9) are solved, it is possible to calculate solutions to the Eqs. (1) using the Eqs. (4) and (5). If the Eqs. (9) do not have a solution, then this method is not possible, since Eq. (7) in that case is an invalid condition.

One-Parameter Group of Transformations of Solutions

Assuming that the functions g_1, \dots, g_6 and the generators A_t and A_x have been determined, one may search for groups transforming solutions of Eqs. (2) into their like. The generator U of such a transformation group requires:

$$\begin{aligned} [U, A_t] &= \lambda_1 A_t + \lambda_2 A_x \quad \text{and} \\ [U, A_x] &= \lambda_3 A_t + \lambda_4 A_x, \end{aligned} \quad (10)$$

where λ_i ($i = 1, \dots, 4$) depends on a_k ($k = 1, 2, \dots, 6$). From a previous treatment [3] of the model we know that:

$$U^r = a_2 \frac{\partial}{\partial a_1} - a_1 \frac{\partial}{\partial a_2}$$

is a generator for space independent solutions of Eqs. (1) with $R=0$. Moreover, it is a generator in

the space-dependent case with $R=0$ and $D_1 = D_2 = D$. To verify this, U^r has to be once-extended [9] with respect to time and space to act in the space of a_i .

$$\begin{aligned} U_{tx}^r &= a_2 \frac{\partial}{\partial a_1} - a_1 \frac{\partial}{\partial a_2} + a_4 \frac{\partial}{\partial a_3} - a_3 \frac{\partial}{\partial a_4} \\ &\quad + a_6 \frac{\partial}{\partial a_5} - a_5 \frac{\partial}{\partial a_6}. \end{aligned} \quad (11)$$

The generator:

$$\begin{aligned} U_{txx}^r &= a_2 \frac{\partial}{\partial a_1} - a_1 \frac{\partial}{\partial a_2} + a_4 \frac{\partial}{\partial a_3} - a_3 \frac{\partial}{\partial a_4} \\ &\quad + a_7 \frac{\partial}{\partial a_8} - a_8 \frac{\partial}{\partial a_7} \end{aligned}$$

which is once-extended with respect to time and twice-extended with respect to space leaves the Eqs. (1) invariant with respect to their form. The parameters $a_7 = \partial^2 c_1 / \partial x^2$ and $a_8 = \partial^2 c_2 / \partial x^2$ have to be substituted in Eqs. (1) to verify this. It may be mentioned that also the generators $\partial/\partial t$ and $\partial/\partial x$ leave Eqs. (1) invariant.

Degeneracy of Infinitesimal Generators

The generators A_t , A_x , and U_{tx}^r can be cast into matrix form:

$$\begin{pmatrix} A_t \\ A_x \\ U_{tx}^r \end{pmatrix} = \begin{pmatrix} a_3 & a_4 & g_1 & g_2 & g_3 \\ a_5 & a_6 & g_3 & g_4 & \frac{1}{D_1}(a_3 - F_1) \\ a_2 & -a_1 & a_4 & -a_3 & a_6 \end{pmatrix} \begin{pmatrix} g_4 \\ \frac{1}{D_2}(a_4 - F_2) \\ -a_5 \end{pmatrix} \begin{pmatrix} \partial/\partial a_1 \\ \partial/\partial a_2 \\ \partial/\partial a_3 \\ \partial/\partial a_4 \\ \partial/\partial a_5 \\ \partial/\partial a_6 \end{pmatrix}. \quad (12)$$

If the generators become linear dependent, then the system of the three generators is degenerated. Firstly, we investigate the case where $A_t = \lambda A_x$. It follows that all 2×2 determinants of the first two rows in the matrix of the right-hand side of Eq. (12) vanish. Hence, using:

$$\lambda = w/k$$

we obtain:

$$\begin{aligned} a_3 &= \frac{w}{k} a_5; \quad a_4 = \frac{w}{k} a_6, \\ g_1 &= \frac{w}{k} g_3; \quad g_2 = \frac{w}{k} g_4, \\ g_3 &= \frac{w}{k} \frac{1}{D_1} (a_3 - F_1), \\ g_4 &= \frac{w}{k} \frac{1}{D_2} (a_4 - F_2) \end{aligned} \quad (13)$$

and the degenerate Equations (2):

$$\begin{aligned} \frac{\partial a_1}{\partial t} &= a_3 = \frac{w}{k} a_5 = \frac{\partial a_1}{\partial x} \frac{w}{k}, \\ \frac{\partial a_2}{\partial t} &= a_4 = \frac{w}{k} a_6 = \frac{\partial a_2}{\partial x} \frac{w}{k}, \\ \frac{\partial a_3}{\partial t} &= \frac{w^2}{k^2} \frac{1}{D_1} (a_3 - F_1) = \frac{\partial a_3}{\partial x} \frac{w}{k}, \\ \frac{\partial a_4}{\partial t} &= \frac{w^2}{k^2} \frac{1}{D_2} (a_4 - F_2) = \frac{\partial a_4}{\partial x} \frac{w}{k}, \\ \frac{\partial a_5}{\partial t} &= \frac{w}{k} \frac{1}{D_1} (a_3 - F_1) = \frac{\partial a_5}{\partial x} \frac{w}{k}, \\ \frac{\partial a_6}{\partial t} &= \frac{w}{k} \frac{1}{D_2} (a_4 - F_2) = \frac{\partial a_6}{\partial x} \frac{w}{k}. \end{aligned} \quad (14)$$

The condition $\partial x / \partial t = w/k$ yields the similarity variable:

$$z = wt - kx.$$

Because of the dependence of a_5 and a_6 on a_3 and a_4 , Eqs. (14) reduce to:

$$\begin{aligned} \frac{\partial a_1}{\partial z} &= \frac{a_3}{w}, \quad \frac{\partial a_3}{\partial z} = \frac{w}{D_1 k^2} (a_3 - F_1), \\ \frac{\partial a_2}{\partial z} &= \frac{a_4}{w}, \quad \frac{\partial a_4}{\partial z} = \frac{w}{D_2 k^2} (a_4 - F_2), \end{aligned} \quad (15)$$

where the similarity variable z is used as a parameter. The generator:

$$\begin{aligned} A_z &= \frac{a_3}{w} \frac{\partial}{\partial a_1} + \frac{a_4}{w} \frac{\partial}{\partial a_2} + \frac{w}{D_1 k^2} (a_3 - F_1) \\ &\quad \cdot \frac{\partial}{\partial a_3} + \frac{w}{D_2 k^2} (a_4 - F_2) \frac{\partial}{\partial a_4} \end{aligned} \quad (16)$$

belongs to the Equations (15). The group U_{tx}^* reduces to

$$U_z = a_2 \frac{\partial}{\partial a_1} - a_1 \frac{\partial}{\partial a_2} + a_4 \frac{\partial}{\partial a_3} - a_3 \frac{\partial}{\partial a_4}.$$

A_z and U_z degenerate to $A_z = \lambda_z U_z$ if

$$\begin{aligned} w \lambda_z &= S, \quad a_3 = S a_2, \\ a_4 &= -S a_1, \quad E - D k^2 \lambda_z^2 = a_1^2 + a_2^2 \end{aligned}$$

admitting under Eqs. (15) the solution:

$$\begin{aligned} a_1 &= (E - D k^2) \cos z, \\ a_2 &= -(E - D k^2) \sin z, \end{aligned} \quad (17)$$

where

$$w = S \quad \text{and} \quad \lambda_z = 1$$

which represents a propagating wave whose amplitude is dependent on the wave number k .

Now the case is studied where

$$U = \lambda_t A_t + \lambda_x A_x \quad \text{and} \quad A_t \neq \lambda A_x.$$

Consequently, all determinants of the three-row matrix in Eqs. (12) are zero. Whereas in the former case the conditions (13) lead to equations which are independent of the unknown functions g_i , the conditions here contain these functions.

$$\begin{aligned} \text{(a)} \quad & \lambda_t a_3 + \lambda_x a_5 + a_2 = 0, \\ \text{(b)} \quad & \lambda_t a_4 + \lambda_x a_6 - a_1 = 0, \\ \text{(c)} \quad & \lambda_t g_1 + \lambda_x g_3 + a_4 = 0, \\ \text{(d)} \quad & \lambda_t g_2 + \lambda_x g_4 - a_3 = 0, \\ \text{(e)} \quad & \lambda_t g_3 + \frac{\lambda_x}{D} (a_3 - F_1) + a_6 = 0, \\ \text{(f)} \quad & \lambda_t g_4 + \frac{\lambda_x}{D} (a_4 - F_2) - a_5 = 0. \end{aligned} \quad (18)$$

Equations (a) and (b) determine λ_t and λ_x and Eqs. (c) through (f) g_1, g_2, g_3 and g_4 . Equations (18) have to be compatible with Equations (8). In general, no functions g_i will satisfy both sets of equations. However, Eqs. (18) may be considered as boundary conditions to Eqs. (8), if they are regarded as sets of partial differential equations in the independent variables x and t . In that case, hypersurfaces in the parameter space may exist

on which both sets are valid. The similarity variable $z = wt - kx$ is an example of such a surface.

Generalization

We assume that the set of infinitesimal generators A_i ($i = 1, 2, \dots, m$) form a Jacobian complete system [10], i.e.

$$[A_i, A_j] = 0 \quad (i, j = 1, 2, \dots, m), \quad (19)$$

and have a common solution. Moreover, there exist $n - m$ independent common solutions to all A_i where n is the number of variables a_k of the A_i . The differential equation systems of first order associated with the $A_i = \sum_k \eta_{ik} \frac{\partial}{\partial a_k}$ is:

$$\frac{\partial a_k}{\partial t_i} = \eta_{ik} \quad (j, k = 1, 2, \dots, n; i = 1, 2, \dots, m), \quad (20)$$

where η_{ik} depends on a_j . It satisfies the integrability conditions (see Eqs. (3)). Hence, the set of parameters (t_i) constitutes a unique coordinate system to represent the quantities a_k . The solutions of Eqs. (20) can be written as Lie-series:

$$\begin{aligned} a_k(t_i) &= \exp \sum_i (t_i A_i) a_k|_{a_k=a_k^0} \\ &= \sum_{v=0}^{\infty} \frac{1}{v!} \left(\sum_i t_i A_i \right)^v a_k|_{a_k=a_k^0} \end{aligned} \quad (21)$$

where a_k^0 are the initial values of the a_k . Within the domain of t_i , where the series converges, the latter represent single-valued unique functions. Moreover, because of the group properties, the inverse function exists with respect to the $\{t_i\}$.

By successive elimination of the a_k 's from the system (20), systems of partial differential equations with mixed and higher order derivatives are obtained. Conversely, it is possible from a system of partial differential equations to construct systems of first order differential equations of the kind given in Eqs. (20). If the compatibility condition applies to this system, the latter can be treated as previously suggested. Since any complete system [10] can be transformed into a Jacobian complete system, one may construct partial differential equation systems of first order, the solutions of which form more-parameter transformation groups starting with any complete system.

The number p of compatibility equations obtained from a system of m parameters t_i in the n variables

a_k is given by:

$$p = \frac{m(m-1)}{2} \cdot n.$$

Since for $m = 3$ the number of constraint equations already is equal to the number of η_{ik} (compare Eq. (20)), the compatibility conditions strongly restrict the equation set (20) for $m > 3$.

The infinitesimal generator U of a group may be used to transform the generators of the Jacobian complete system A_i by commutation into:

$$A_i^* = [U, A_i].$$

Let λ_{ij} be functions of the variables a_k and

$$A_i^* = \sum_j \lambda_{ij} A_j \quad (i, j = 1, 2, \dots, m),$$

then the new generators A_i^* form a complete system having the same set of common solutions as A_j . Therefore, the group generated by U transforms the set of solutions into themselves, assuming:

$$[U, A_i] = \sum_j \lambda_{ij} A_j \quad (i, j = 1, 2, \dots, m). \quad (22)$$

The transformation from A to A^* does not need to preserve the parameterization, since it uniquely maps solutions into other solutions, but not necessarily the parameter space into itself. The latter would require that the set of $\{A_i^*\}$ also forms a Jacobian complete system. More than one U may have this property (22). The number l of independent U 's has to be less than $n - m + 1$, since otherwise the excessive U 's would be dependent on the other U 's through:

$$U = \sum_{j=1}^m \lambda_j A_j + \sum_{s=1}^{n-m} \mu_s U_s$$

(where λ_j, μ_s are functions of a_k and μ_s common solutions to all A_i).

The main property of the considered set of solutions is the uniqueness inherent to its group character. Consequently, given any initial value, there is only one path connecting neighbouring values (in this case curves or surfaces cannot intersect). The uniqueness is abolished, if the generators of the group degenerate by becoming mutually dependent, e.g.:

$$U = \sum_{j=1}^m \lambda_j A_j. \quad (23)$$

The set of values for which the uniqueness does not apply can be considered as singular. This set may

be regarded as the boundary of a domain in which uniqueness is valid.

A differential equation system of first order:

$$\frac{\partial}{\partial \tau_s} a_k = u_{sk} \quad (\tau_s \text{ are parameters}) \quad (24)$$

belongs to any independent

$$U_s = \sum_s u_{sk} \frac{\partial}{\partial a_k} \quad (\text{see (20)}).$$

Eqs. (20) and (24) form a differential equation system in $m+1 \geq n$ parameters (t_i, τ_s) , which does not necessarily satisfy the compatibility conditions.

So far, uniqueness in the description has been the major topic. Another property of the physical laws is the independence of the coordinate system. In the following, we restate the former quality in the vector space notation [11] to stress its invariance with respect to coordinate transformations. In this notation, an infinitesimal generator is a vector field which assigns a vector to each point in space. Here, the vectors $a = (a_1, a_2 \dots a_n)$ with $(a \in M_a)$ constitute a manifold M_a (the space) to which the vectors $A_i \in T_a$ are assigned. T_a is the vector space of tangents at $a \in M_a$ whose basis is given by

$$\left\{ \frac{\partial}{\partial a_k} \quad (k = 1, 2, \dots, n) \right\}.$$

The η_{ik} (see Eq. (20)) is the vector component in the space of tangents. Multilinear maps, which map elements of a vector space onto the corresponding field, are called tensors. Alternating tensors form subspaces of tensor spaces, which are distinguished by their high symmetry. The alternating tensors of the tangent space are called forms. The basis of the vector space of one-forms is $\{da_k\}$. The basis of h -forms can be expressed by the wedge product of the basis of one-forms, e.g. a 3-form has the basis:

$$\{da_k \wedge da_i \wedge da_j \quad (k > i > j; k, i, j = 1, 2, \dots, n)\}.$$

A particular form is the n -form (the volume element) w :

$$w = w(a_k) da_1 \wedge da_2 \wedge \dots \wedge da_n.$$

The following three operations are defined in the vector space of forms: $L_x \alpha$, dx , and $X \lrcorner \alpha$, where L_x is the Lie derivative of the form α with respect to the vector field X of the corresponding tangent

space. The symbol d is the exterior derivative of the form α and $X \lrcorner \alpha$ is the contraction of α with X .

Note that contraction converts a h -form into a $(h-1)$ -form whereas an exterior derivation changes an h -form into an $(h+1)$ -form.

Let $w(a_k) = 1$, then w is the unit volume element. By contraction of w with vector fields, one obtains the $(n-1)$ -forms:

$$\begin{aligned} \alpha_i &= A_i \lrcorner w \quad (i = 1, 2, \dots, m), \\ \mu &= U \lrcorner w. \end{aligned}$$

The condition $[U, A_i] = \lambda_{ij} A_j$ can now be rewritten as:

$$L_U \alpha_i = \lambda_{ij}' \alpha_j \quad (i, j = 1, 2, \dots, m).$$

Thus, in coordinate-free form for

$$\begin{aligned} \text{Eqs. (12): } L_{A_i} \alpha_j &= 0, \\ \text{Eqs. (22): } L_U \alpha_i &= \sum \lambda_{ij}' \alpha_j, \\ \text{Eqs. (23): } U \lrcorner \beta &= 0, \end{aligned} \quad (25)$$

where $i, j = 1, 2, \dots, m$ and

$$\begin{aligned} \alpha_j &= A_j \lrcorner w \quad \text{and} \\ \beta &= A_1 \lrcorner (A_2 \lrcorner \dots \lrcorner (A_m \lrcorner w) \dots) \end{aligned}$$

are obtained.

The parameters (t_i, τ_s) can also form a manifold with the associated tangent space T_τ . The basis of T_τ is given by

$$\left\{ \frac{\partial}{\partial t_i}, \quad \frac{\partial}{\partial \tau_s} \quad (i = 1, 2, \dots, m; s = 1, 2, \dots, l) \right\}.$$

The dual space has the basis $\{dt_i, d\tau_s\}$.

The dimension of the combined tangent spaces is maximally equal to $2n$. The description of the physical processes may also be made in this combined space [12].

Canonical Form of Groups and Coordinate Transformations

Groups of transformations with more than one continuous parameter are produced by a generator U , which admits the representation:

$$U = e_1 U_1 + e_2 U_2 + \dots + e_r U_r,$$

where e_i is a real constant and the U_i ($i = 1, 2, \dots, r$) forms a system of independent generators. The parameter r is the number of continuous variables.

Multi-parameter groups may be classified according to distinct relations, established by the Grassman (or Lie) algebra [13] of commutators and their independent generators. The two-parameter (t, x) -example admits the classification of two-parameter groups. There are four classes [10] (I)–(IV), satisfying the following conditions:

$$\begin{aligned} \text{(I)} \quad & [U_1, U_2] = 0, \quad U_2 \neq \varrho U_1, \\ \text{(II)} \quad & [U_1, U_2] = 0, \quad U_2 = \varrho U_1, \\ \text{(III)} \quad & [U_1, U_2] = U_1, \quad U_2 \neq \varrho U_1, \\ \text{(IV)} \quad & [U_1, U_2] = U_1, \quad U_2 = \varrho U_1, \end{aligned} \quad (26)$$

where ϱ is a function of the variables of the U 's.

The generators of the classes (I) and (II) of Eqs. (26) are given in the canonical variables u_1 and u_2 by:

$$\begin{aligned} \text{(I)} \quad & U_1 = \partial/\partial u_1, \quad U_2 = \partial/\partial u_2, \\ \text{(II)} \quad & U_1 = \partial/\partial u_2, \quad U_2 = u_1 \partial/\partial u_2. \end{aligned} \quad (27)$$

The commutator vanishes for both classes, i.e. they form a Jacobian complete system.

Changing to new variables a_i by the transformation:

$$a_i = a_i(u_1, u_2) \quad (i = 1, 2, \dots, n)$$

leads to the generators U_1^* , U_2^* according to [10]:

$$\begin{aligned} U_1^* &= \sum_{i=1}^n (U_1 a_i) \frac{\partial}{\partial a_i}; \\ U_2^* &= \sum_{i=1}^n (U_2 a_i) \frac{\partial}{\partial a_i}. \end{aligned}$$

Evidently, the commutator of the generators U_1^* and U_2^* vanishes, i.e.

$$[U_1^*, U_2^*] = 0$$

since it is preserved under coordinate transformations. Hence, U_1^* and U_2^* also form a Jacobian complete system. In the same manner, Jacobian complete systems may be constructed from canonical forms of multi-parameter groups with more than two parameters. In turn, these Jacobian complete systems may be used as described in the previous section.

Discussion

The criteria developed for limit cycles in a previous paper [3] may, as the example shows, be extended to systems involving spatial coordinates. A one-parameter group may still be found which transforms solutions of the defining differential equations into their like. The process of transformation becomes singular if the solution is an invariant function of the group. Invariant functions are transformed into themselves by the transformations of the group. Thus, solutions which are symmetrical with respect to the one-parameter group reveal the special properties of limit cycles. They are independent of the parameter that transforms solutions into new solutions. Since the parameters, which fix a solution, are initial and boundary data, the symmetrical solution is independent of some of these data.

In a multi-dimensional case, the condition of symmetry severely restricts the solutions. Therefore, a solution requires a prescribed boundary in the parameter space (x, t) . This phenomenon may be interpreted as structure generation in the space of parameter variables. Some processes of morphogenesis in biology [14] might be explained by such phenomenon. In this context, it should be mentioned that the compatibility conditions also greatly restrict the set of models allowed. Moreover, they strongly constrain the space of parameter variables (x, t) for dimensions greater than three. Since compatibility is closely related to Lie-algebras, the models may be arranged according to the classification of the associated Lie-algebra.

The preceding sections only treat dynamical aspects of chemical or similar models. The latter are often related to the thermodynamics of irreversible processes. The structural and energetic views of thermodynamics would supply additional characteristics. Particularly the boundary operation would implicate new useful relations.

Finally, we emphasize that the description outlined is not restricted to chemical networks, but may also be applied to systems of other species and quantities. Systems generating discrete parameter groups are probably of considerable interest for analysis, e.g. of interacting biological systems.

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