Symmetries of S-Systems

EBERHARD O. VOIT
Department of Biostatistics, Epidemiology, and Systems Science, Medical University of South Carolina, Charleston, South Carolina

Received 4 March 1991; revised 21 August 1991

ABSTRACT

An S-system is a set of first-order nonlinear differential equations that all have the same structure: The derivative of a variable is equal to the difference of two products of power-law functions. S-systems have been used as models for a variety of problems, primarily in biology. In addition, S-systems possess the interesting property that large classes of differential equations can be recast exactly as S-systems, a feature that has been proven useful in statistics and numerical analysis. Here, simple criteria are introduced that determine whether an S-system possesses certain types of symmetries and how the underlying transformation groups can be constructed. If a transformation group exists, families of solutions can be characterized, the number of S-system equations necessary for solution can be reduced, and some boundary value problems can be reduced to initial value problems.

INTRODUCTION

Polynomials and rational functions might appear to provide the simplest nonlinear mathematical structures for the modeling of nonlinear dynamic processes. However, models based on these functions become mathematically intractable as soon as phenomena with moderately high numbers of components and interactions are investigated (cf. [10, p. 85f]). An alternative is the power-law formalism. This formalism is based on linear approximation in logarithmic space, which leads to a set of differential equations that is known as an *S-system* [9, 14, 18, 21]. An S-system with n dependent variables X_i and one independent variable t is defined as

$$\frac{dX_i}{dt} = \alpha_i \prod_{j=1}^{n} X_j^{g_{ij}} - \beta_i \prod_{j=1}^{n} X_j^{h_{ij}}, \qquad i \in \{1, \ldots, n\},$$

where the dependent variables and the constants α_i and β_i are nonnegative, and the exponents g_{ij} and h_{ij} are real.

655 Avenue of the Americas, New York, NY 10010 0025-5564/92/$05.00

The S-system representation offers many theoretical and practical advantages for the analysis of complicated networks and has found applications in various areas, including biochemistry, genetics, immunology, cell biology, forestry, and economics. These applications are too numerous to be discussed here but have been reviewed elsewhere several times (e.g., [10], [15], [18]).

In addition to their use as approximate representations of complicated phenomena, S-systems possess the interesting property that large classes of ordinary differential equations can be *recast* exactly as S-systems (e.g., [15], [18], [23]). Typically the number of variables increases when a system is recast, but through algebraic constraints on the new initial conditions the behavior of the resulting S-system is restricted to a manifold of the same dimension as the original problem. The recasting of differential equations as S-systems offers a number of advantages:

(1) Functions and differential equations can be objectively compared and classified, because recast as S-systems they differ only in parameter values and not in structure. For instance, the biological literature contains a large number of growth functions that can produce almost indistinguishable graphs but show no similarity in their functional forms. Upon recasting, they differ merely in some of their parameter values [11, 12, 17, 22].

(2) The S-system classification of functions can be used to generalize or optimize functional forms. For instance, if growth data are being analyzed but the underlying growth function is not known, the S-system formulation can help to identify this function (cf. [17]).

(3) Recast as S-systems, differential equations can often be solved faster than with standard software [3, 4, 15].

(4) Complicated functions sometimes can be evaluated more efficiently in S-system form; examples that have been elaborated in some detail include noncentral probability distributions (e.g., [8], [20]).

The following analysis shows that elementary operations are sufficient to determine whether an S-system admits symmetries that are characterized by groups of translation or scaling. If so, a particular analytical or numerical solution gives rise to an entire family of solutions. Furthermore, the number of S-system equations necessary for solution can be reduced, and some types of boundary value problems reduce to initial value problems.

LOCAL LIE GROUPS OF COORDINATE TRANSFORMATIONS

In some differential equations the independent and dependent variables can be subjected to transformations and nevertheless the differential equations remain unaltered or *invariant*. In such a situation, the equation is said to *admit the transformation*. Although very general types of transformations are possible, applications are often concerned with translation, scaling, or rotation. A simple example is the scaling transformation of the homogeneous equation

$$\frac{dy}{dx} = \frac{x^2 + y^2}{xy}.$$

It is not difficult to see that x and y can be transformed to $x_1 = px$, $y_1 = py$ ($p \in \mathbb{R}_+$), and the differential equation in x_1 and y_1 has the same form as the equation in x and y:

$$\frac{dy_1}{dx_1} = \frac{x_1^2 + y_1^2}{x_1 y_1}.$$

When p is written as $\exp(\varepsilon)$, the set of all transformations of this type form an additive group in the parameter ε [2]. Some differential equations admit several independent transformations of this type, thus representing n-parameter groups. The following theorem provides criteria for the existence and construction of transformation groups for dynamical systems represented in S-system form.

THEOREM 1. LIE GROUPS OF SCALING TRANSFORMATIONS OF QUASI-HOMOGENEOUS S-SYSTEMS

Let

$$\frac{dX_i}{dX_0} = \alpha_i \prod_{j=0}^{n} X_j^{g_{ij}} - \beta_i \prod_{j=0}^{n} X_j^{h_{ij}}, \qquad i \in \{1, \ldots, n\}, \tag{1}$$

be a potentially nonautonomous S-system with explicit incorporation of the independent variable X_O. Let G be an $n \times (n+1)$ matrix with elements

$$G_{ij} = \begin{cases} g_{ij} + 1 & \text{if } \alpha_i \neq 0 \text{ and } j = 0, \\ g_{ij} & \text{if } \alpha_i \neq 0 \text{ and } j \neq i, \\ g_{ij} - 1 & \text{if } \alpha_i \neq 0 \text{ and } j = i, \\ 0 & \text{if } \alpha_i = 0, \end{cases} \tag{2}$$

where $i = 1, \ldots, n$ and $j = 0, \ldots, n$. Let H_{ij} be defined analogously with h and β instead of g and α. Let (C_{ij}) be the $2n \times (n+1)$ matrix whose first n rows contain G_{ij} and whose remaining rows contain H_{ij}. Let v

be a column vector with $n+1$ real components $v_O, v_1, \ldots, v_n$ and $\mathbf{o}$ the zero $(2n)$-vector. Let p be a positive real number.

(i) If the system

$$(C_{ij})\boldsymbol{v} = \mathbf{o} \tag{3}$$

has a nontrivial solution $\boldsymbol{v} = (v_o, v_1, \ldots, v_n)^T$, then the transformations

$$Y_j = p^{v_j} X_j, \qquad j = 0, \ldots, n;\ p \in \mathbb{R}_+ \tag{4}$$

form a one-parameter Lie group of coordinate transformations that leaves the S-system (1) *unaltered. That is, the equation is invariant under the group.*

(ii) Let

$$\rho = \operatorname{rank}(C_{ij}) \tag{5}$$

and let $\{\boldsymbol{v}_k\}$ be a set of $n+1-\rho$ linearly independent solutions to (3). *Let $\boldsymbol{v}_k$ have the components v_{kj}. Then* (1) *admits the $(n+1-\rho)$-dimensional Lie group of transformations,*

$$Y_j = \prod_{k=1}^{r} p_k^{v_{kj}} X_j, \tag{6}$$

with $r = n+1-\rho$ parameters $p_1, p_2, \ldots, p_r \in \mathbb{R}_+$.

Remark 1. The groups in (i) and (ii) are called *stretching groups* or *scaling groups*, and S-system (1) is said to be *quasi-homogeneous* when it admits such groups (cf. [1]).

Remark 2. For $r > 1$, a one-parameter group of transformations of type (4) can be generated from the r transformations (6) by setting $p = p_1 = p_2 = \cdots = p_r$.

Remark 3. A similar theorem holds if the differential equations in (1) contain more than two terms [18, Ch. 15].

Proof. (i) Condition (3) is equivalent to the two conditions

$$v_i - v_0 = \sum_{j=0}^{n} v_j g_{ij}, \qquad \alpha_i \neq 0, \tag{7a}$$

and

$$v_i - v_0 = \sum_{j=0}^{n} v_j h_{ij}, \qquad \beta_i \neq 0, \tag{7b}$$

$i = 1, \dots, n$. If $\alpha_i = 0$ or $\beta_i = 0$, the corresponding parts of (3) are trivially satisfied. From (4) and (7) we obtain the differential equations for Y_i,

$$\begin{aligned}
\frac{dY_i}{dY_0} &= \frac{dY_i}{dX_i}\frac{dX_i}{dX_0}\frac{dX_0}{dY_0} = p^{v_i}\frac{dX_i}{dX_0}p^{-v_0} \\
&= p^{v_i - v_0}\left[\alpha_i \prod_{j=0}^{n}\left(p^{-v_j}Y_j\right)^{g_{ij}} - \beta_i \prod_{j=0}^{n}\left(p^{-v_j}Y_j\right)^{h_{ij}}\right] \\
&= p^{v_i - v_o}\left[p^{-\sum_{j=0}^{n} v_j g_{ij}}\alpha_i \prod_{j=0}^{n} Y_j^{g_{ij}} - p^{-\sum_{j=0}^{n} v_j h_{ij}}\beta_i \prod_{j=0}^{n} Y_j^{h_{ij}}\right] \\
&= \alpha_i \prod_{j=0}^{n} Y_j^{g_{ij}} - \beta_i \prod_{j=0}^{n} Y_j^{h_{ij}},
\end{aligned}$$

which holds because of (7). Under composition, the transformations (4) form a one-parameter group with the identity transformation $Y_i = X_i$ when $p = 1$ and the inverse transformation $Y_i = (1/p)^{v_i} X_i$; closure and associativity are obvious.

(ii) If system (3) has two or more linearly independent solutions, then each solution $\boldsymbol{v}_k$ corresponds to a transformation

$$Y_{kj} = p^{v_{kj}} X_j, \qquad j = 0, \dots, n;\ k = 1, \dots, n+1-\rho, \tag{8}$$

and composition of these transformations generates transformations of type (6).

The transformations (6) leave the S-system (1) unaltered. As in part (i), we have for all $k \leqslant r$ and $\alpha_i \neq 0$, $\beta_i \neq 0$, $i = 1, \dots, n$,

$$v_{ki} - v_{k0} = \sum_{j=0}^{n} v_{kj} g_{ij} \tag{9a}$$

and

$$v_{ki} - v_{k0} = \sum_{j=0}^{n} v_{kj} h_{ij}. \tag{9b}$$

The differential equations for the new variables Y_i then are

$$\begin{aligned}\frac{dY_i}{dY_0} &= \prod_{k=1}^{r} p_k^{v_{ki}} \frac{dX_i}{dX_0} p_k^{-v_{ko}} \\ &= \prod_{k=1}^{r} p_k^{v_{ki}-v_{ko}} \prod_{j=0}^{n} \left(\prod_{m=1}^{r} p_m^{-v_{mj}} \right)^{g_{ij}} \alpha_i \prod_{j=0}^{n} Y_j^{g_{ij}} - \beta\text{-term} \\ &= \prod_{k=1}^{r} p_k^{v_{ki}-v_{ko}-\sum_{j=0}^{n} v_{kj} g_{ij}} \alpha_i \prod_{j=0}^{n} Y_j^{g_{ij}} - \beta\text{-term} \\ &= \alpha_i \prod_{j=0}^{n} Y_j^{g_{ij}} - \beta_i \prod_{j=0}^{n} Y_j^{h_{ij}},\end{aligned}$$

where the β-term is transformed in the same fashion as the α-term. Thus, the r-parameter transformation (6) leaves the S-system (1) unaltered.

The linear independence of transformations of type (8) is evident when one defines c_k such that $p^{c_k} = p_k$ and rewrites Equation (6) as

$$Y_j = p^{\sum_{k=1}^{r} c_k v_{kj}} X_j,$$

where $r = n + 1 - \rho$. Thus, under composition the collection of one-parameter groups (8) generates an $(n + 1 - \rho)$-dimensional Lie group of transformations of type (6) with the identity transformation $Y_j = X_j$ when $p_k = 1$ for all k, and the inverse transformation $Y_j = \Pi_k (1/p_k)^{v_{kj}} X_j$; closure and associativity again are obvious.

Example. Consider the S-system

$$\frac{dX_1}{dX_0} = X_1^2 X_2^{-1} X_3 - X_1^{1/2} X_2^{1/2} X_3^{-1/2} \tag{10a}$$

$$\frac{dX_2}{dX_0} = X_2 \qquad - X_1^{2/3} X_2^{1/3} X_3^{2/3} \tag{10b}$$

$$\frac{dX_3}{dX_0} = X_1 X_2^{-1} X_3^2 - X_3. \tag{10c}$$

The matrix (C_{ij}) is

$$\begin{pmatrix} 1 & 1 & -1 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 1 & -1 & 1 \\ 1 & -1/2 & 1/2 & -1/2 \\ 1 & 2/3 & -2/3 & 2/3 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

which reduces to

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & -1 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

with rank $\rho = 2$ and solution $v_0 = 0$, $v_1 = c_1$, $v_2 = c_2$, $v_3 = c_2 - c_1$ with arbitrary real c_1 and c_2.

Specifying $c_1 = c_2 = 1$, we obtain

$$Y_{11} = p_1 X_1, \qquad Y_{12} = p_1 X_2, \qquad Y_{13} = X_3, \qquad p_1 \neq 0. \tag{11}$$

Alternatively, specifying $c_1 = 0$, $c_2 = 1$, we obtain

$$Y_{21} = X_1, \qquad Y_{22} = p_2 X_2, \qquad Y_{23} = p_2 X_3, \qquad p_2 \neq 0. \tag{12}$$

The c-vectors span the solution space. It is easily verified that both transformations (11) and (12) and the compound transformation

$$Y_1 = p_1 X_1, \qquad Y_2 = p_1 p_2 X_2, \qquad Y_3 = p_2 X_3 \tag{13}$$

leave the original S-system (10) unaltered.

APPLICATIONS

Theorem 1 allows us to determine transformations of coordinates that leave the set of S-system differential equations unaltered. These transformations can be employed in different ways. Five applications are (1) reduction in the number of equations necessary for solution, (2) determination of transformation groups for differential equations not in S-system form, (3) lowering the order of differential equations, (4) determination of other types of transformation groups, and (5) solution of some boundary value problems. In addition to these applications, which are discussed in the following, transformations of coordinates can be helpful in computing analytical solutions of S-systems and of steady states of S-systems in which some α_i or β_i equal zero [18, Ch. 15].

REDUCTION IN THE NUMBER OF SYSTEM EQUATIONS

One way to perform this reduction is to determine group invariants and use them as the new coordinates (e.g., [2]). In general, group invariants are functions of the system variables that are unaltered by the action of the group. As an example, for the scaling group $G^1:(x, y) \mapsto (\lambda x, \lambda y)$ with $\lambda > 0$, the function $\zeta(x, y) = x/y$ is an invariant defined on the upper and lower half-planes $\{y \neq 0\}$ [6, p. 80]. For the S-system (1), the most obvious group invariants have the form

$$\xi_i = \prod_{k=0}^{n} X_k^{s_{ik}},$$

where the exponents s_{ik} satisfy the condition

$$\sum_{k=0}^{n} v_k s_{ik} = 0,$$

which is derived directly from the definition of group invariants and from (7):

$$\begin{aligned} \xi_i(Y_1, \dots, Y_n) &= \prod_{k=0}^{n} Y_k^{s_{ik}} = \prod_{k=0}^{n} \left(p^{v_k} X_k\right)^{s_{ik}} = p^{\Sigma v_k s_{ik}} \prod_{k=0}^{n} X_k^{s_{ik}} \\ &= \xi_i(X_1, \dots, X_n). \end{aligned}$$

The most convenient functionally independent set of group invariants presumably is

$$\xi_i = X_i X_n^{-v_i/v_n}, \tag{14}$$

$i = 0, \dots, n-1$, with the additional definition

$$\xi_n = X_n$$

because the inverse of this transformation, which is needed to retrieve the original variables from the reduced system, is easily determined to be

$$X_i = \xi_i \xi_n^{v_i/v_n}, \qquad X_n = \xi_n.$$

As an alternative to (14), or in the case of $v_n = 0$, one can select another index j with $v_j \neq 0$ and employ the invariants

$$\xi_i = X_i X_j^{-v_i/v_j}$$

or one can renumber the equations such that $v_n \neq 0$.

Representing the original S-system (1) in terms of the new variables ξ_i, as defined in (14), and using (7), we obtain for $i = 0, \dots, n-1$, and

$v_0 \neq 0$,

$$\xi_n^{v_0/v_n} \frac{d\xi_i}{dX_0} = \alpha_i \prod_{k=0}^{n-1} \xi_k^{g_{ik}} - \beta_i \prod_{k=0}^{n-1} \xi_k^{h_{ik}} - \alpha_n \frac{v_i}{v_n} \xi_i \prod_{k=0}^{n-1} \xi_k^{g_{nk}} + \beta_n \frac{v_i}{v_n} \xi_i \prod_{k=0}^{n-1} \xi_k^{h_{nk}}. \tag{15}$$

If $v_0 = 0$, then $\xi_0 = X_0$, and Equation (15) reduces to

$$\frac{d\xi_i}{d\xi_0} = \alpha_i \prod_{k=0}^{n-1} \xi_k^{g_{ik}} - \beta_i \prod_{k=0}^{n-1} \xi_k^{h_{ik}} - \alpha_n \frac{v_i}{v_n} \xi_i \prod_{k=0}^{n-1} \xi_k^{g_{nk}} + \beta_n \frac{v_i}{v_n} \xi_i \prod_{k=0}^{n-1} \xi_k^{h_{nk}}. \tag{16}$$

For $v_0 \neq 0$, one divides Equations (15) for $i = 1, \ldots, n-1$ by the equation of $d\xi_0/dX_0$.

In either case, ξ_n does not appear on the right-hand side of the resulting equation. Thus, the system can be solved without the equation for ξ_n, while ξ_n itself is determined in a second step by quadrature (cf. [6, p. 158f]). Specifically, ξ_n is obtained from the S-system equation of X_n ($= \xi_n$) in (1) upon substitution of the new variables ξ_i for the old variables X_i. For $v_0 = 0$, the result is the separable equation

$$\frac{d\xi_n}{d\xi_0} = \xi_n \left[\alpha_n \prod_{k=0}^{n-1} \xi_k^{g_{nk}} - \beta_n \prod_{k=0}^{n-1} \xi_k^{h_{nk}} \right].$$

For $v_0 \neq 0$, $d\xi_n/d\xi_0$ also is separable, but the expression in brackets is divided by the right-hand side of (15) for $i = 0$.

If any of the variables ξ_i does not appear on the right-hand side, the system can be reduced further, for the remaining equations can be solved without the equation for ξ_i. Furthermore, if ξ_0 only appears in the equation of $d\xi_0/dX_0$, the system can be reduced either by elimination of the equation of $d\xi_0/X_0$ or by selecting a new invariant ξ_j as differentiation variable and expressing the system in the form $d\xi_i/d\xi_j$. Many of these reductions will be exemplified later with the Blasius equation.

It is interesting to note that the reduced set (16) has the form of a so-called *generalized mass action system* (cf. [15] and [18, Ch. 12]) or *multinomial system* (cf. [7]) whose right-hand sides consist of arbitrary sums and differences of products of power-law functions and not just one positive and one negative term as in the S-system structure. In a sense, the reduction in the number of equations can be seen as the reverse procedure of recasting generalized mass action systems as S-systems (cf. [18, Ch. 15]).

Lowering the number of equations is of mathematical significance and may have computational implications. It also can help to detect redundancies in S-system models by revealing allometric (power-law) relationships among the system variables. Transformation of coordinates is not the only way to lower the number of equations; alternatives include the computation of trajectorial solutions and the solution of related partial differential equations [18, Ch. 15].

DIFFERENTIAL EQUATIONS NOT IN S-SYSTEM FORM

In combination with the techniques for recasting differential equations exactly as S-systems [15], symmetries of systems other than S-systems can be analyzed. For instance, the second-order equation

$$\ddot{Z} = Z^{-1}\dot{Z}^2 - 2[1+\ln(t)]t^{-2}Z$$

is recast by introduction of the S-system variables $X_0 = t$, $X_1 = 1+\ln(t)$, $X_2 = Z$, $X_3 = dZ/dt$, and subsequent differentiation (cf. [15]). The resulting S-system is

$$\frac{dX_1}{dX_0} = X_0^{-1}, \qquad \frac{dX_2}{dX_0} = X_3,$$

$$\frac{dX_3}{dX_0} = X_2^{-1}X_3^2 - 2X_0^{-2}X_1X_2,$$

which admits transformations of the type $v_0 = v_1 = 0$, $v_2 = v_3$. Consequently, scaling Z and dZ/dt by the same factor leaves the second-order differential equation unaltered.

LOWERING THE ORDER OF DIFFERENTIAL EQUATIONS

As an example, let's analyze the Blasius equation whose symmetry properties were recently discussed in some detail by Schwarz [16]. The Blasius equation is a third-order ordinary differential equation of the form

$$y''' = b\ y\ y'',$$

where b is a real parameter. To rewrite the equation in S-system form, we define $X_0 = x$, $X_1 = y$, $X_2 = y'$, and $X_3 = y''$. The S-system and the corresponding matrix (C_{ij}) then are

$$\frac{dX_1}{dX_0} = X_2, \qquad \frac{dX_2}{dX_0} = X_3, \qquad \frac{dX_3}{dX_0} = bX_1X_3,$$

and

$$\begin{pmatrix} 1 & -1 & 1 & 0 \\ 1 & 0 & -1 & 1 \\ 1 & 1 & 0 & 0 \end{pmatrix}.$$

Straightforward application of Theorem 1 leads to the one-parameter transformation

$$Z_0 = p^{-c}X_0, \qquad Z_1 = p^c X_1,$$
$$Z_2 = p^{2c}X_2, \qquad Z_3 = p^{3c}X_3.$$

The order of the Blasius equation or, equivalently, the number of equations of the S-system analog, can be reduced in different ways, leading to different simplifications. As examples we consider direct application of Equation (15), employment of a reduction variable different from ξ_n, and the trivial transformation given by $c = 0$.

(1) For $c \neq 0$ and thus $v_0 \neq 0$, application of Equation (15) yields

$$\xi_3^{-1/3}\frac{d\xi_0}{dX_0} = 1 + \frac{1}{3}b\xi_0\xi_1,$$

$$\xi_3^{-1/3}\frac{d\xi_1}{dX_0} = \xi_2 - \frac{1}{3}b\xi_1,$$

$$\xi_3^{-1/3}\frac{d\xi_2}{dX_0} = 1 - \frac{2}{3}b\xi_1\xi_2.$$

Since ξ_0 only appears in the equation of $d\xi_0/dX_0$, the second and third equations can be solved without ξ_0. Specifically, division of the third equation by the second yields the single first-order differential equation

$$\frac{d\xi_2}{d\xi_1} = \frac{3 - 2b\xi_1\xi_2}{3\xi_2 - b\xi_1}.$$

(2) As an alternative to selecting ξ_n for reduction, we can choose another invariant ξ_j. Let's select ξ_0. The new coordinates then are

$$\xi_1 = X_0X_1, \qquad \xi_2 = X_2X_0^2, \qquad \xi_3 = X_3X_0^3.$$

Based on these invariants, different reduced systems can be obtained, depending on the value of the parameter c.

For $c \neq 0$, the system in new coordinates, according to Equation (15), becomes

$$\xi_0 \frac{d\xi_1}{dX_0} = \xi_1 + \xi_2,$$

$$\xi_0 \frac{d\xi_2}{dX_0} = 2\xi_2 + \xi_3,$$

$$\xi_0 \frac{d\xi_3}{dX_0} = b\xi_1\xi_3 + 3\xi_3,$$

from which the solution in new coordinates is immediately obtained as

$$\frac{d\xi_2}{d\xi_1} = \frac{2\xi_2 + \xi_3}{\xi_1 + \xi_2}, \qquad \frac{d\xi_3}{d\xi_1} = \frac{b\xi_1\xi_3 + 3\xi_3}{\xi_1 + \xi_2}.$$

Identifying $u = xy = \xi_1$, $v = x^2 y' = \xi_2$, $x^3 y'' = \xi_3$, one obtains Schwarz's [16] equation (40).

For the degenerate case, $c = 0$, a set of invariants is $\xi_i = X_i$, $i = 1, \ldots, 3$, and reduction yields

$$\frac{d\xi_2}{d\xi_1} = \frac{\xi_3}{\xi_2}, \qquad \frac{d\xi_3}{d\xi_1} = b\frac{\xi_1\xi_3}{\xi_2}.$$

Using Schwarz's [16, p. 461] notation ($u = y = \xi_1$, $v = y' = \xi_2$, $a = -b$), differentiation and substitution directly yield the second-order differential equation

$$vv'' + v'^2 + auv' = 0$$

(equation (38) in [16]).

The last equation again has symmetry. Upon recasting the equation as an S-system, the same type of elementary operations as above yield the new variables $u = \xi_1 = yx^{-2}, v = \xi_2 = y'x^{-1}$. Differentiation and substitution produce the first-order differential equation

$$uv'(v - 2u) + v^2 + (a + u)v = 0,$$

which is Schwarz's equation (39).

Employing the S-system representation, all these results were derived with elementary matrix operations, while Schwarz notes that "to find the symmetry group of a differential equation almost always requires tremendous algebraic calculations" and the change in variables "usually involves lengthy calculations."

OTHER TYPES OF TRANSFORMATION GROUPS

The technique of recasting a differential equation as an S-system can be used to detect other types of groups. This will now be demonstrated with the prominent example of translation groups, which can be determined upon logarithmic coordinate transformation. Consider the differential equation

$$\frac{dY}{dX} = a(X - Y)^{-2}.$$

Define new variables as $X_0 = \exp(X)$, $X_1 = \exp(Y)$, which results in

$$\frac{dX_1}{dX_0} = \frac{X_1}{X_0} a[\ln(X_0) - \ln(X_1)]^{-2}.$$

By defining $X_2 = \ln(X_0) - \ln(X_1)$, one obtains the additional S-system equation

$$\frac{dX_2}{dX_0} = X_0^{-1} - aX_0^{-1}X_2^{-2}.$$

The system matrix (C_{ij}) then is

$$\begin{pmatrix} 0 & 0 & -2 \\ 0 & 0 & -1 \\ 0 & 0 & -3 \end{pmatrix}.$$

Evidently, the rank is 1, and the solution corresponds to the transformation

$$Y_0 = p^{\upsilon_0} X_0, \qquad Y_1 = p^{\upsilon_1} X_1, \qquad Y_2 = p^0 X_2,$$

with real υ_0 and υ_1. However, the recasting constraint $X_2 = \ln(X_0) - \ln(X_1)$ must also be satisfied in the new coordinate system; that is, $Y_2 = \ln(Y_0) - \ln(Y_1)$, and thus we require

$$\begin{aligned} Y_2 = X_2 &\stackrel{!}{=} \ln(X_0 p^{-\upsilon_0}) - \ln(X_1 p^{-\upsilon_1}) \\ &= \ln(X_0) + \ln(p^{-\upsilon_0}) - \ln(X_1) - \ln(p^{-\upsilon_1}), \end{aligned}$$

which is satisfied only for $\upsilon_0 = \upsilon_1$. Hence, the S-system variables can be transformed as

$$Y_0 = p^{\upsilon_0} X_0, \qquad Y_1 = p^{\upsilon_0} X_1, \qquad Y_2 = X_2,$$

which corresponds to the translation of the original equation

$$\tilde{Y} = Y + \varepsilon, \qquad \tilde{X} = X + \varepsilon$$

(cf. [2, p. 9]).

By applying the logarithmic transformation to only some of the variables, combinations of stretching and translation can be studied. Consider the pair of differential equations

$$\frac{dX}{dt} = \frac{Y}{(t-X)^2}, \qquad \frac{dY}{dt} = Y^g,$$

where g is a real parameter. First, we determine the stretching groups. We define $X_0 = t$, $X_1 = X$, $X_2 = Y$, $X_3 = t - X$, and obtain the S-system

$$\frac{dX_1}{dX_0} = X_2 X_3^{-2}, \qquad \frac{dX_2}{dX_0} = X_2^g, \qquad \frac{dX_3}{dX_0} = 1 - X_2 X_3^{-2}.$$

The matrix (C_{ij}) is

$$\begin{pmatrix} 1 & -1 & 1 & -2 \\ 1 & 0 & g-1 & 0 \\ 1 & 0 & 0 & -1 \\ 1 & 0 & 1 & -3 \end{pmatrix} \to \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 2g-1 \end{pmatrix}$$

The rank depends on the numerical value of the parameter g. For $g \neq 1/2$, there are no stretching groups. For $g = 1/2$, the rank is 3, and the solution is $v_0 = v_1 = v_3 = c$, $v_2 = 2c$, which corresponds to the one-parameter transformation group

$$Y_0 = p^c X_0, \qquad Y_1 = p^c X_1, \qquad Y_2 = p^{2c} X_2, \qquad Y_3 = p^c X_3,$$

and one verifies directly that the recasting constraint

$$Y_3 = p^c X_3 = p^c(X_0 - X_1) = Y_0 - Y_1$$

is satisfied.

Now we can study translation groups. We define $X_0 = \exp(t)$, $X_1 = \exp(X)$, $X_2 = \exp(Y)$, $X_3 = \ln(X_2) = Y$, $X_4 = \ln(X_0) - \ln(X_1) = \ln(t) - \ln(X)$, and obtain the S-system

$$\frac{dX_1}{dX_0} = \frac{X_1}{X_0} X_3 X_4^{-2}, \qquad \frac{dX_2}{dX_0} = \frac{X_2}{X_0} X_3^g,$$

$$\frac{dX_3}{dX_0} = X_0^{-1} X_3^g, \qquad \frac{dX_4}{dX_0} = X_0^{-1} - X_0^{-1} X_3 X_4^{-2}.$$

The matrix (C_{ij}) is

$$\begin{pmatrix} 0 & 0 & 0 & 1 & -2 \\ 0 & 0 & 0 & g & 0 \\ 0 & 0 & 0 & g-1 & 0 \\ 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 1 & -3 \end{pmatrix},$$

which reduces to

$$\begin{pmatrix} 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

with the solution $v_0 = a$, $v_1 = b$, $v_2 = c$, $v_3 = 0$, and $v_4 = 0$. This result implies that the S-system admits a three-dimensional Lie group of transformations, given by $p_1 = p^a$, $p_2 = p^b$, $p_3 = p^c$. However, checking the constraints that were introduced by recasting the original system in S-system form, we find, for $p \neq 1$,

$$\begin{aligned} Y_4 = X_4 &= \ln(X_0) - \ln(X_1) = \ln(Y_0) - \ln(Y_1) + \ln(p^{-a}) - \ln(p^{-b}) \\ &= \ln(Y_0) - \ln(Y_1) \qquad \text{iff } a = b \end{aligned}$$

and

$$Y_3 = p^0 X_3 = \ln(p^{-c} Y_2) = \ln(Y_2) \qquad \text{iff } c = 0.$$

Hence, the three-dimensional group is constrained to a one-dimensional subgroup corresponding to

$$\begin{aligned} Y_0 &= p^a X_0 = p^a \exp(t) = \exp(t + \tau), \\ Y_1 &= p^a X_1 = p^a \exp(X) = \exp(X + \tau), \\ Y_2 &= X_2 = \exp(Y). \end{aligned}$$

Stretching and translating combined, the original equation remains invariant under the transformation

$$Z_0 = p^c(t + \tau), \qquad Z_1 = p^c(X + \tau), \qquad Z_2 = p^{2c} Y.$$

Straightforward calculation confirms the result:

$$\frac{dZ_1}{dZ_0} = \frac{dZ_1}{dX}\frac{dX}{dt}\frac{dt}{dZ_0} = p^c\frac{dX}{dt}p^{-c}$$

$$= \frac{p^{-2c}Z_2}{\left(p^{-c}Z_0 - \tau - p^{-c}Z_1 + \tau\right)^2} = \frac{Z_2}{\left(Z_0 - Z_1\right)^2},$$

$$\frac{dZ_2}{dZ_0} = p^{2c}\frac{dY}{dt}p^{-c} = p^c\left(p^{-2c}Z_2\right)^g = Z_2^{1/2}, \qquad g = 1/2.$$

BOUNDARY-VALUE PROBLEMS

The fact that entire families of solutions satisfy an S-system in favorable cases can be used to solve boundary-value problems. Intuitively, it may be the easiest to imagine an autonomous S-system with two dependent variables X_1 and X_2 and boundary values given at t_1 and t_2. If the S-system admits a transformation that affects X_2 but leaves X_1 unchanged [i.e., $v_1 = 0$, $v_2 \neq 0$ in (4)], one can solve the system initialized at t_1 with the correct initial value $X_1(t_1)$ and a guess for $X_2(t_1)$. As the admitted transformation does not affect $X_1(t)$, one can scale the trial solution of X_2 in such a way that it produces the correct boundary value at t_2.

In more general terms, consider an S-system with boundary values $X_i(t_i)$, instead of initial values $X_i(t_1)$ that admits a one-parameter group. Symbolically or numerically compute the solution $Y_i(t)$ of the corresponding initial-value problem $X_i(t_1)$. If the admitted transformation has the form $Z_i = p^{v_i}X_i$ and if there exists a number $c \in \mathbb{R}$ such that the trial solution $Y_i(t)$ of the initial-value problem and the true solution $X_i(t)$ of the boundary-value problem satisfy the conditions $Y_i(t_i) = p^{c \cdot v_i}X_i(t_i)$, $i = 0, \ldots, n$, then the true solution $X_i(t)$ can be computed from the trial solution $Y_i(t)$ of the initial-value problem.

Typically, the particular trial solution $Y_i(t)$ determines whether or not the above conditions are satisfied. However, given a favorable symmetry structure of the S-system, the boundary-value problem can always be computed. For example, the boundary-value problem

$$\frac{dX_1}{dX_0} = X_1X_2X_3 - X_1, \qquad \frac{dX_2}{dX_0} = X_2^2X_3 - X_2, \qquad \frac{dX_3}{dX_0} = -X_3,$$

$X_1(10) = 1$, $X_2(5) = 1$, $X_3(5) = 1$, leads to a matrix (C_{ij}) that reduces to

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

with rank 2 and solution $v_0 = 0$, $v_1 \in \mathbb{R}$, $v_2 + v_3 = 0$. A numerical trial solution, initiated at $t_0 = 5$ with $Y_i(5) = 1$, $i = 1, \ldots, 3$, produces $Y_1(10) = 0.001347$. This suggests a transformation with $p^{v_0} = 1$, $p^{v_1} = 1/0.001347$, $p^{v_2} = 1$, $p^{v_3} = 1$, which yields $X_1(5) = 1/0.001347$, $X_2(5) = Y_2(5) = 1$, $X_3(5) = Y_3(5) = 1$. With these conditions, at $t_0 = 5$, the problem is reduced to an initial-value problem that produces the entire solution.

Other boundary-value problems that can be addressed deal with networks in which some of the boundary values can be chosen. An example of such a problem is the task to select X_1 and X_2 at time t_0 in such a way that X_3 and X_4 at time points t_1 and t_2 produce desired boundary values.

CONCLUSION

The detection of symmetries and their associated local Lie groups of coordinate transformations is essential for the algebraic characterization and general solution of nonlinear differential equations. Since the fundamental work of Lie (e.g., [5]), many authors have attacked the problem of finding transformation groups; during the past two decades especially, interest in this important area of differential equations has been awakened again (cf. [16]).

Although many factors contribute to the difficulty of detecting symmetries, one intrinsic problem of nonlinear differential equations is that not only do they differ in their parameter values, as linear differential equations do, but they also differ with respect to their structure. This individuality in structure makes every nonlinear differential equation special and often prevents us from developing methods of analysis that are general enough to be applicable to even moderately large classes of equations.

The S-system structure provides a canonical form that, via recasting, contains very many differential equations as special cases. This embedding of nonlinear functions into one unifying form offers analytical, numerical, and practical advantages and allows their objective comparison, classification, and generalization (e.g., [13], [14], [17], [18]). It also makes it possible to detect common features of the recast nonlinearities that may not have been visible in their original formulation and facilitates the determination of optimal functional forms. For instance, the search for the distribution function that best models actual data reduces to a parameter estimation problem, once all relevant distribution functions are recast as S-systems (cf. [13], [19]). A comprehensive computer program, ESSYNS, was developed for the analysis of S-systems [4, 24]. This program exploits the homogeneous S-system structure and, as a consequence, computes numerical solutions and various steady-state properties with considerably higher efficiency than any other available algorithms.

The symmetry analysis presented here demonstrates that recasting a nonlinear differential equation as an S-system can also help to elucidate its fundamental algebraic properties. Once recast as an S-system, the evaluation of groups of coordinate transformations is reduced to straightforward, simple matrix algebra. This is especially interesting because virtually any ordinary differential equation can be recast and the recasting process itself requires only elementary operations. As recasting and the determination of transformation groups are both based on simple rules, they probably could be implemented in symbolic algebra programs, which would make the analysis of symmetries even more efficient.

I am grateful to Dr. Donald C. Lewis for his extraordinary patience in answering questions and improving the manuscript. I also thank Dr. Lawrence Dresner for some key ideas in the applications section and Dr. Philip Rust for his valuable, constructive criticisms. This work was in part supported by grant 2RO1 GM30054-05 of the National Institutes of Health.

REFERENCES

1 V. I. Arnold, *Geometrical Methods in the Theory of Ordinary Differential Equations,* Springer-Verlag, New York, 1983.

2 J. M. Hill, *Solution of Differential Equations by Means of One-Parameter Groups,* Pitman, Boston, 1982.

3 D. H. Irvine, Efficient solution of nonlinear models expressed in S-system canonical form, *Math. Comput. Modelling* 11:123–128 (1988).

4 D. H. Irvine and M. A. Savageau, Numerical solution of nonlinear ordinary differential equations expressed in canonical forms, *SIAM J. Num. Anal.* 27:704–735 (1990).

5 S. Lie, *Vorlesungen über Differentialgleichungen mit bekannten infinitesimalen Transformationen,*, B. G. Teubner, Leipzig, 1891 (reprint: Chelsea, New York, 1967).

6 P. J. Olver, *Applications of Lie Groups to Differential Equations,* Springer-Verlag, New York, 1986.

7 M. Peschel and W. Mende, *The Predator–Prey Model: Do We Live in a Volterra World?,* Akademie-Verlag, Berlin, 1986.

8 P. F. Rust and E. O. Voit, Statistical densities, cumulatives, quantiles, and power obtained by S-system differential equations, *J. Am. Stat. Assoc.* 85(410):572–578 (1990).

9 M. A. Savageau, Biochemical systems analysis, I. Some mathematical properties of the rate law for the component enzymatic reactions, *J. Theor. Biol.* 25:365–369 (1969).

10 M. A. Savageau, *Biochemical Systems Analysis: A Study of Function and Design in Molecular Biology,* Addison-Wesley, Reading, Mass., 1976.

11 M. A. Savageau, Growth of complex systems can be related to the properties of their underlying determinants, *Proc. Natl. Acad. Sci. USA* 76:5413–5417 (1979).

12 M. A. Savageau, Growth equations: a general equation and a survey of special cases, *Math. Biosci.* 48:267–278 (1980).

13 M. A. Savageau, A suprasystem of probability distributions, *Biom. J.* 24:323–330 (1982).
14 M. A. Savageau and E. O. Voit, Power-law approach to modeling biological systems; I. Theory, *J. Ferment. Technol.* 60(3):221–228 (1982).
15 M. A. Savageau and E. O. Voit, Recasting nonlinear differential equations as S-systems: a canonical nonlinear form, *Math. Biosci.* 87:83–115 (1987).
16 F. Schwarz, Symmetries of differential equations: from Sophus Lie to computer algebra, *SIAM Rev.* 30:450–481 (1988).
17 E. O. Voit, S-system analysis of endemic infections, *Comput. Math. Appl.* 20(4–6):161–173 (1990).
18 E. O. Voit, ed., *Canonical Nonlinear Modeling: S-System Approach to Understanding Complexity,* Van Nostrand Reinhold, New York, 1991.
19 E. O. Voit and H. J. Anton, Derivation of the frequency distribution of cycle durations from continuous-labeling curves, *J. Theor. Biol.* 112:575–588 (1985).
20 E. O. Voit and P. F. Rust, Evaluation of the noncentral t distribution with S-systems, *Biom. J.* 32(6):681–695 (1990).
21 E. O. Voit and M. A. Savageau, Power-law approach to modeling biological systems; III. Methods of analysis, *J. Ferment. Technol.* 60(3):233–241 (1982).
22 E. O. Voit and M. A. Savageau, Analytical solutions to a generalized growth equation, *J. Math. Anal. Appl.* 103(2):380–386 (1984).
23 E. O. Voit and M. A. Savageau, Equivalence between S-systems and Volterra-systems, *Math. Biosci.* 78:47–55 (1986).
24 E. O. Voit, D. H. Irvine, and M. A. Savageau, *The User's Guide to ESSYNS,* Medical University of South Carolina Press, 1989.