# How many variables? Some comments on the dimensionality of nonlinear systems

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Abstract. While at first glance seemingly obvious, the number of variables in a model is not a priori fixed. For mathematical purposes, it is oftentimes convenient to reduce the number of variables to a minimum, but such reduction sometimes obscures meaning and insight and is not always computationally optimal. This is demonstrated with a special class of nonlinear differential equations, called *S-systems*, whose specific mathematical structure makes reduction as well as expansion of models translucent. The reduction shown here is based on the determination of *Lie groups of scaling transformations*, while the expansion is based on equivalent recasting. The Lie reduction constitutes the inverse operation to the recasting of multinomial systems.

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## 1. Introduction

At first glance, the number of variables in a model seem to be one of the best defined quantities. In contrast to parameter values or the mathematical forms of the governing processes, which often are insufficiently characterized or not known at all, the first step in designing a model is the listing of its constituents. Hence, almost by definition the number of variables is given. Nevertheless, at second thought the number of variables can be argued on two grounds. One derives from the subject area of the modeled phenomenon, and the other is an issue of mathematical representation. While there may be some overlap between the two, the distinction is easy to intuit.

Subject Area. Only in clear-cut cases is the number of variables beyond question. Even in prototype models, such as those describing the dynamics in predatorprey systems, modelers and ecologists are likely to argue about alternative prey, competing predators, and other contributors to the ecosystem of which the investigated predator-prey pair is just one part. In biochemical systems analysis, the modeler has to decide which compounds are biochemically and functionally similar enough to allow their aggregation in mathematically homogeneous pools that are represented by single variables. In organismic phenomena like growth, the key variables are certain high-lever measurements like weights or volumes or organs, whereas molecular and biochemical aspects are usually not explicitly represented. The number of variables, thus, depends on the organizational level at which a model is constructed. By including certain components and excluding others, the model focuses on some aspects of the phenomenon and ignores others. For instance, the classical infectious disease models that, with a total of three variables, account for susceptible, infected, and removed individuals, by virtue of this definition exclude aspects of age and sex. It is obvious that the number of necessary or desired variables, in the end, is a compromise between actuality with respect to the subject area and mathematical tractability. Model reduction in this sense has been discussed extensively in the literature and is not subject of this report.

Mathematical representation. In contrast to model reduction or expansion within the subject area, mathematical reduction and expansion deal with equivalent representations. In this case, the organizational level of the model has been determined and is not subject to further discussion. The question asked now is *Is it possible to find mathematical transformations that allow us to characterize certain properties of the model more efficiently, for instance, by decoupling simultaneous differential equations?* As we shall see in the following, this question can have many answers, depending on the criteria chosen to evaluate competing representations. In some cases, constraints or conservation laws can be used to uncouple equations, in other cases, it actually turns out to be advantageous to increase the number of variables and equations. I shall demonstrate some scenarios as they come up in S-system models, without claiming exhaustiveness.

# 2. Transformations that affect the number of simultaneous equations

**2.1. Reduction in number.** Under opportune circumstances, various general and *ad hoc* methods are available to reduce the number of differential equations that is necessary for solution. For instance, if a constraint is known that allows a system variable  $X_i$  to be expressed as a function of another system variable  $X_j$ , then  $X_i$  can be substituted with this function, and the differential equation for  $X_i$  is no longer necessary to solve for the remaining variables and can be eliminated. If  $X_i$  is of interest, it can be computed in a separate step from  $X_j$ . From a mathematical standpoint, this "decoupling" usually simplifies the original problem. Decoupling can be accomplished in two ways. In the first case, the resulting system is exactly equivalent to the original; I will discuss an example of such a transformation in this report. In the second case, equations with different time scales are decoupled from each other by considering the slow equations to be in steady state (e.g., [4, 8]).

A second well-known reduction in the number of equations applies to autonomous systems. Under favorable conditions, the independent variable can be eliminated by expressing the dependent variables  $X_2, X_3, \ldots$  in terms of  $X_1$ , which is accomplished by dividing the equations for  $X_2, X_3, \ldots$  by the equation for  $X_1$ . The result is a non-autonomous "trajectorial" system with one equation less than the original system.

A method that seems to be appreciated only by a select group of experts is the determination of *Lie groups of coordinate transformations*. If such groups can be found, the number of simultaneous equations can be reduced. Furthermore, knowledge of such groups elucidates the structure of the differential equation by showing which quantities are invariant under the action of the group. The invariants can often be interpreted in terms of conservation laws, such as the conservation of mass and energy in closed systems. Lie group analysis in general is rather difficult. In the special case of scaling transformations in S-systems, however, the analysis can be executed with means of elementary linear algebra. The following states conditions for the existence of such Lie groups and demonstrates how they can be employed in the analysis of models in S-system form.

The general ideas of transformation groups and invariants may best be illustrated with a simple example. Consider the differential equation

$$\frac{dy}{dx} = \frac{x^2 y^2}{x^4 - y^4}.$$
(2.1)

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

$$\frac{dy_1}{dx_1} = \frac{x_1^2 y_1^2}{x_1^4 - y_1^4}.$$
(2.2)

When p is written as  $exp(\epsilon)$ , the set of all transformations of this type form an additive group in the parameter  $\epsilon$ . If a differential equation admits several (say k) independent transformations of this type, it admits a k-parameter group.

While the identification of transformation groups in general is quite complicated, scaling transformations of S-systems are characterized with elementary methods: One simply constructs a particular matrix from the kinetic order parameters  $g_{ij}$  and  $h_{ij}$ . If the rank of this matrix is not maximal, the S-system admits a Lie group of transformations. Specifically, let

$$\frac{dX_i}{dX_0} = \alpha_i \prod_{j=0}^n X_j^{g_{ij}} - \beta_i \prod_{j=0}^n X_j^{h_{ij}} \quad i = 1, 2, \dots, n$$
(2.3)

be a potentially non-autonomous S-system with explicit incorporation of the independent variable  $X_0$ . Let  $\mathcal{G}$  be an  $(n \times (n+1))$  matrix with elements

$$\mathcal{G}_{ij} = \begin{cases} g_{ij} + 1 & \text{if } \alpha_i \neq 0 \text{ and } j = 0, \\ g_{ij} & \text{if } \alpha_i \neq 0 \text{ and } j \neq i, \\ g_{ij} - 1 & \text{if } \alpha_i \neq 0 \text{ and } j = i, \\ 0 & \text{if } \alpha_i = 0, \end{cases}$$
(2.4)

where i = 1, ..., n and j = 0, ..., n. Let  $\mathcal{H}_{ij}$  be defined analogously with h and  $\beta$  instead of g and  $\alpha$ . Let  $\mathcal{C}$  be the  $(2n \times (n+1))$  matrix whose first n rows contain  $\mathcal{G}_{ij}$  and whose remaining rows contain  $\mathcal{H}_{ij}$ . Let  $\vec{v}$  be a column vector with n + 1 real components  $v_0, v_1, v_2, ..., v_n$ , and  $\vec{o}$  the zero (2n)-vector. Let p be a positive real number.

(i) If the system

$$\mathcal{C}\vec{v} = \vec{o} \tag{2.5}$$

has a non-trivial solution  $\vec{v} = (v_0, v_1, v_2, \dots, v_n)^{tr}$ , the the transformations

$$Y_j = p^{v_j} X_j \quad j = 0, \dots, n; \quad p \in \mathcal{R}$$

$$(2.6)$$

form a one-parameter Lie group of coordinate transformations that leaves the S-system Eq. (2.3) unaltered. That is, the equation is invariant under the group.

(ii) Let

$$\rho = rank(\mathcal{C}) \tag{2.7}$$

and let  $\vec{v}_1, \vec{v}_2, \ldots, \vec{v}_r$  be a set of  $r = n+1-\rho$  linearly independent solutions to Eq. (2.5). Let  $\vec{v}_k$  have the components  $v_{kj}$ . Then eq. (2.3) admits the *r*-dimensional Lie group of transformations

$$Y_{j} = \prod_{k=1}^{r} p_{k}^{v_{kj}} X_{j}$$
(2.8)

with r parameters  $p_1, p_2, \ldots, p_r \in \mathcal{R}_+$ . The proof of (i) and (ii) can be found in [10].

#### Remarks.

1) The groups in (i) and (ii) are called *stretching groups* or *scaling groups*, and S-system (2.3) is called *quasi-homogeneous* when it admits such groups.

2) For r > 1, a one-parameters group of transformations of type (2.6) can be generated from the r transformations (2.8) by setting  $p = p_1 = p_2 = \ldots = p_r$ .

3) A similar theorem holds if the differential equations in Eq. (2.3) contain more than two terms [9, Ch. 15].

If an S-system admits a Lie group of transformations, the number of simultaneous equations necessary for solution can be reduced. This is accomplished by determine *group invariants*, which are functions of the original system variables that remain unaltered by the action of the group. The most convenient, functionally independent set of group invariants in our case is

$$\xi_i = X_i X_n^{-\nu_i/\nu_n} \quad i = 0, \dots, n-1$$
(2.9)

$$\xi_n = X_n, \tag{2.10}$$

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

$$X_i = \xi_i \xi_n^{\nu_i/\nu_n} \tag{2.11}$$

$$X_n = \xi_n. \tag{2.12}$$

As an alternative to Eqns. (2.9) and (2.10), or in the case of  $v_n = 0$ , one can select another index j with  $v_j \neq 0$  and employ the invariants

$$\xi_i = X_i X_j^{-\nu_i/\nu_j} \tag{2.13}$$

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

Other applications of the Lie-group analysis shown above include the lowering of the order of a differential equation (e.g., [10]), the analytical computation of steady-states in S-systems that lack some production or degradation terms [9:, Ch. 15], and, in favorable cases, the analytical solution of S-systems [9: Ch. 15]. As an illustration, the next section gives an example that has relevance to modeling.

**Example. A boundary value problem in Pharmacodynamics.** Janszen [3] has recently formulated physiologically-based pharmacokinetic models within the framework of S-systems. These models describe how a drug upon injection or inhalation is distributed through an organism over a period of time. Janszen showed that S-system models with parameter values determined from physiological measurements, such as transport rates and partition coefficients, accurately describe the dynamics of drug concentrations in various organs and plasma over time. His model for the pharmacodynamics of the antibiotic sulfathiazole in swine reads

$$X_{i} = \alpha_{i}X_{6} - \beta_{i}X_{i} \quad i = 1, \dots, 5$$
$$\dot{X}_{y} = \alpha_{6}\prod_{j=1}^{5} X_{j}^{g_{6j}} - \beta_{6}X_{6}.$$
(2.14)

The variables  $X_i$  represent various organs or tissues,  $X_6$  represents plasma. According to the rules for setting up an S-system model, the structure of Janszen's model immediately shows that all flow of drug is facilitated by ways of plasma. Note that, independent of their numerical values, the exponents  $g_{ij}$  in the sixth equation always sum up to 1, because the S-system model was designed in such a way that it behaved exactly like a traditional compartment model at a desired operating point. Specifically, if the sum of linear terms is approximated by a powerlaw term, the exponents in this term add up to 1. Given this model and initial values, the dynamical responses of all concentrations are readily computed with numerical methods. However, questions of the following type are difficult to answer: Given that the plasma concentration of the drug at time  $t^*$  is  $X_p(t^*)$ , how much of the drug was given at time t = 0? Assuming that all drug concentrations, except that of plasma, were zero at time 0, the question poses a boundary value problem that, a priori, is difficult to solve. Lie group analysis can be employed to address the problem.

The first step is construction of the matrix C from the exponents  $g_{ij}$  and  $h_{ij}$  of the S-system model. We stack up Janszen's matrix of g's

	/ 0	0	0	0	0	1
ĺ	0	0	0	0	0	1
	0	0	0	· 0	0	1
	0	0	0	0	0	1
	0	0	0	0	0	1
	0	0	0	0	0	1
	0.24004	0.34087	0.28842	0.08370	0.04697	0/

and the matrix of h's

	/1	0	0 0 1 0 0	0	0	0\	
ĺ	0	1	0	0	0	0	
	$ \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} $	0 1 0 0 0	1	0	0	0	
	0	0	0	1	0	0	,
	0	0	0	0	1	0	
	0/	0	0	0	0	1/	

add a zero-th column with all 1's, and subtract 1 from all  $g_{ii}$  and  $h_{ii}$ . The resulting matrix is thus  $12 \times 7$ . Its reduction to row echelon form is executed with the usual matrix operations of linear algebra. First, we observe that the diagonal elements of the former matrix of h's disappear, resulting in six rows of the form  $(1 \ 0 \ 0 \ 0 \ 0 \ 0)$ . This row is subtracted from the first six rows. Then, we add 0.24004 times the first row, 0.34087 times the second row, etc. to the sixth row. This reduces the sixth row to a row of 0's, since the exponents  $g_{ij}$  in the sixth model equation sum up to 1. Upon renumbering rows, the result is the matrix

$$C = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & -1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$
 (2.15)

The rank of the matrix is (n + 1) - 1, which indicates that the model admits a one-parameter stretching group.

Solution of the equation

$$\mathcal{C}\vec{v} = \vec{o} \tag{2.16}$$

yields  $v_0 = 0$ ,  $v_i = v_j$   $(i, j \neq 0)$ , and when we use  $v_6 \neq 0$  as reference, the new coordinates are

$$\xi_0 = X_0 = t$$
  

$$\xi_i = X_i X_6^{-v_i/v_6} \quad (i = 1, \dots, 5)$$
  

$$\xi_6 = X_6.$$
  
(2.17)

The model in new coordinates is obtained by differentiation and substitution of  $\xi_i$  for  $X_i$ :

$$\frac{d\xi_i}{d\xi_0} = \dot{\xi_i} = \frac{\dot{X_i}X_6 - X_i\dot{X_6}}{X_6^2}.$$
(2.18)

For instance, one obtains for the first variable

$$\dot{\xi}_i = \alpha_1 - \beta_1 X_1 X_6^{-1} - \alpha_6 X_1 X_6^{-2} \prod_{j=1}^5 X_j^{g_{6j}} - \beta_6 X_1 X_6^{-1}, \qquad (2.19)$$

which reduces to

$$\dot{\xi}_i = \alpha_1 - \beta_1 \xi_1 - \alpha_6 \xi_1 \prod_{j=1}^5 \xi_j^{g_{6j}} - \beta_6 \xi_1$$
(2.20)

since the  $g_{6j}$  sum to 1. Note that this equation, just like the second through fifth equations, does not contain  $\xi_6$ . In other words, the first five equations can be solved without consideration of the sixth. The equation for  $\xi_6$ ,

$$\dot{\xi}_6 = \xi_6 [\alpha_6 \prod_{j=1}^5 \xi_j^{g_{6j}} - \beta_6 \prod_{j=1}^5 \xi_j^{h_{6j}}], \qquad (2.21)$$

is separable and can be solved once the solution of the first five equations has been obtained.

What is the bottom line result of this analysis? After transformation to a new coordinate system, the model now is expressed in variables  $\xi_i = X_i/X_6$ , which are interpretable as *relative* drug concentrations (with respect to plasma concentration). In other words, the model is independent of the absolute magnitudes of concentrations. Furthermore, we are able to reduce the boundary value problem to an initial value problem. This is done in the following way:

- 1. Initialize system at time 0 with  $X_i = 0$   $(i = 1, ..., 5), X_6 = 1$ .
- 2. Solve system up to point  $t^*$ .
- 3. Solve system again, this time initialized at time 0 with  $X_i = 0$  (i = 1, ..., 5),  $X_6 = X_{6-computed}(t^*) / X_{6-observed}(t^*)$ . Because of its scaling property, indicated by the Lie group, the system satisfies the boundary value problem.

**2.2. Increase in number.** Minimality is often considered a criterion of optimality when it comes to mathematical representation. As early as in the 14th century, this idea was explicitly formulated by William of Ockham who postulated that between two alternative theories with the same explanatory power the more "parsimonious" theory should be judged better (in: [12]). While condensation of representation in many cases in indeed desirable, mathematics has also encountered precedents and compelling arguments against this notion. Two well established cases are higher-order differential equations and the realization of a proper rational transfer function in the form of a linear time-invariant dynamical equation [1: p. 154f]. In the well-known first case, new variables are introduced for higher derivatives, and the original *n*-th order equation is replaced by a set of *n* first-order equations. In the second case, the input-output description of a system with *p* input terminals and *q* output terminals is

$$\vec{y}(t) = \int_{t_0}^t \mathcal{G}(t,\tau) \vec{u}(\tau) d\tau \qquad (2.22)$$

where  $\vec{y}$  is the  $q \times 1$  output vector,  $\vec{u}$  is the  $p \times 1$  input vector, and  $\mathcal{G}$  is the  $q \times p$  impulse-response matrix of the system. This system description is equivalently represented as

$$\vec{x} = \mathcal{A}(t)\vec{x}(t) + \mathcal{B}(t)\vec{u}(t)$$
(2.23)

$$\vec{y}(t) = \mathcal{C}(t)\vec{x}(t) + \mathcal{E}(t)\vec{u}(t), \qquad (2.24)$$

where  $\vec{x}$  is the  $n \times 1$  state vector of the system, and  $\mathcal{A}$ ,  $\mathcal{B}$ ,  $\mathcal{C}$ , and  $\mathcal{E}$  are timedependent matrices of appropriate dimension. Specifically, if  $\hat{\mathcal{G}}$  in the frequency domain is a scalar function of the type

$$\hat{g}(s) = e + \frac{\beta_1 s^{n-1} + \ldots + \beta_{n-1} s + \beta_n}{s^n + \alpha_1 s^{n-1} + \ldots + \alpha_{n-1} s + \alpha_n}$$
(2.25)

the realization of  $\hat{g}(s)$  is

$$\begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \vdots \\ \dot{x}_{n-1} \\ \dot{x}_n \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 & \dots & 0 & 0 \\ 0 & 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & 1 \\ -\alpha_n & -\alpha_{n-1} & -\alpha_{n-2} & \dots & -\alpha_2 & -\alpha_1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_{n-1} \\ x_n \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix} u$$

$$y = (\beta_n \quad \beta_{n-1} \quad \beta_{n-2} \quad \dots \quad \beta_2 \quad \beta_1) \overrightarrow{x} + e \overrightarrow{u}$$
(2.26)

(cf. [1]). That is, one (integral) equation (for y(t)) is replaced by n differential equations.

The method of recasting. *Recasting* is a further example for the advantages of non-minimal representations. Recasting is a method for representing differentiable functions and differential equations as S-systems. This equivalent transformation

is typically accompanied by an increase in the number of independent variables. The following paragraphs list the standard recasting methods, discuss some of the advantages of recast representations, and finally show relationships between recasting and system reduction via Lie transformation groups.

Given a differential equation, it is initially not at all obvious how to obtain an equivalent representation in S-system form. Nonetheless, a standard recasting process has been developed [6] that always succeeds, even though it may not yield optimal results. This process consists of three types of operations which, in a given situation, may have to be applied several times: (i) decompose composite functions; (ii) translocate non-positive variables to the positive real domain; and (iii) reduce sums of products of power-law functions to a single difference between products of power-law functions. In particular cases, *ad hoc* transformations are possible and often preferable (e.g., [9, 11]). The process is best illustrated with an example.

Example. Blue Sky Catastrophes. The system

$$\dot{x} = 0.7y + x - 10xy^{2}$$
$$\dot{y} = C - x + 0.25\sin(1.5t)$$
(2.27)

describes an apparently almost-periodic solution, but in some cases unexpectedly begins to grow without bound, generating a so-called *blue sky catastrophy* (cf. [7]).

The first step of the recasting process is to assure positivity of all variables. To this end, we introduce the variables  $X_1 = x + p$ ,  $X_2 = y + q$ ,  $X_3 = \sin(1.5t) + r$ , and  $X_4 = \cos(1.5t) + r$ . Differentiation yields

$$\dot{X}_{1} = [10pq^{2} - 0.7q - p] - [10q^{2} - 1]X_{1} - [20pq - 0.7]X_{2} + 20qX_{1}X_{2} - X_{1}X_{2}^{2} + 10pX_{2}^{2}$$
$$\dot{X}_{2} = 0.25X_{3} - X_{1}$$
$$\dot{X}_{3} = 1.5X_{4} - 1.5r$$
$$\dot{X}_{4} = 1.5r - 1.5X_{2}$$
(2.28)

In this representation, p and q can be chosen freely, as long as they are large enough to assure positivity, and r is given as r = 4(C + p); for a typical value of C = 0.097 (eg., [7]), one may choose p = q = 10, r = 40.388.

To obtain the S-system form, the first equation, which is in so-called *multinomial* form, replace the variable  $X_1$  with the product of three new variables. For instance, we may specify  $X_1 = X_5^2 X_6^2 X_7^2$ , where powers of two have been chosen for illustration purposes. Differentiation of  $X_1$  leads to the sum  $2\dot{X}_5 X_5 X_6^2 X_7^2 + 2\dot{X}_6 X_5^2 X_6 X_7^2 + 2\dot{X}_7 X_5^2 X_6^2 X_7$ . Equate the first positive plus the first negative power-law term of the first equation with  $2\dot{X}_5 X_5 X_6^2 X_7^2$ , the second positive plus the second negative power-law term of the first equation with  $2\dot{X}_6 X_5^2 X_6 X_7^2$ , and the remaining two terms with  $2\dot{X}_7 X_5^2 X_6^2 X_7$ .

The result without renumbering is

$$X_2 = 0.25X_3 - X_5^2 X_6^2 X_7^2 \quad X_2(t_0) = y(t_0)$$

$$\dot{X}_{3} = 1.5X_{4} - 60.582 \quad X_{3}(t_{0}) = \sin(1.5t_{0}) + r$$

$$\dot{X}_{4} = 60.582 - 1.5X_{3} \quad X_{4}(t_{0}) = \cos(1.5t_{0}) + r$$

$$\dot{X}_{5} = 4991.5X_{5}^{-1}X_{6}^{-2}X_{7}^{-2} - 499.5X_{5} \quad X_{5}(t_{0}) = x(t_{0})^{0.5}$$

$$\dot{X}_{6} = 100X_{2}X_{6} - 999.65X_{2}X_{5}^{-2}X_{6}^{-1}X_{7}^{-2} \quad X_{6}(t_{0}) = 1$$

$$\dot{X}_{7} = 50X_{2}^{2}X_{5}^{-2}X_{6}^{-2}X_{7}^{-1} - 5X_{2}^{2}X_{7} \quad X_{7}(t_{0}) = 1.$$
(2.29)

For a numerical example with  $x(t_0) = y(t_0) = 9.6$ , the initial vector is (9.6, 40.388, 41.388, 9.6<sup>0.5</sup>, 1, 1). The original variables x and y are recouped as  $x = X_5^2 X_6^2 X_7^2 - p$  and  $y = X_2 - q$ .

Advantages of recasting. The recasting process transforms differential equations into S-systems that usually have more equations but a simpler structure than the original equations. The regularity of the resulting system can be exploited for efficient numerical analysis. In particular, Irvine and Savageau [2] have shown that the S-system form allows recursive computation of Taylor series expansions which are the basis for a robust and efficient numerical integrator. Such an algorithm has been implemented in the software ESSYNS, and it has been demonstrated with numerous benchmark tests [2, 6] that in very many cases the computational effort created by the increase in size is recouped, and that systems are often computed faster and with higher accuracy when they are recouped, and that systems re often computed faster and with higher accuracy when they are recast as S-systems.

Recasting can be employed as a tool for the classification and optimization of functional forms. For instance, Savageau [5] has shown that all prominent growth functions are special cases of a two-variable S-system. This form facilitates the search for the growth law that would best model a set of data: Instead of comparing different functional forms, one merely optimizes parameter values of the recast system. Similarly, probability density functions have been recast and classified. Their S-system representation allowed evaluations, such as the computation of quantiles, that in the original form are often complicated (cf. [11]).

Recasting can also be used as modeling tool, when a complex phenomenon is to be represented as an S-system model but some subsystems are not in S-system form [9: Ch. 14]. For instance, an ecological model may significantly depend on the circadian change in solar radiation. The required inclusion of an appropriate oscillation would destroy the S-system form and prevent us from using many of the established symbolic or numerical S-system methods of analysis. In such a situation it is helpful to recast the oscillation and thus to regain the S-system form.

**Relationship between Lie-group analysis and recasting.** Since recasting typically increases the number of variables and equations, one may ask whether it is possible to reverse the recasting process and to reduce a recast S-system to a lower-dimensional system in non-S-system form. In general, this "decasting"

process requires solution of partial differential equations or some semi-systematic trial and error (cf. [9: Ch. 15]). However, there are two notable exceptions. First, if the recasting procedure itself is known, decasting is trivial since one just substitutes back the functions for the auxiliary variables. Second, if the recasting process had included the reduction of multinomial equations, decasting is possible *via* Lie group analysis. This becomes evident from a comparison of the recasting process and the method of decoupling equations in S-systems admitting a Lie-group.

For the recasting a multinomial system as an S-system one substitutes the variable  $X_i$  with the product of two new variables,  $X_i = X_{n+1}X_{n+2}$ , which may be raised to some powers, and replaces the differential equation for  $X_i$  with equations for  $X_{n+1}$  and  $X_{n+2}$ .

On the other hand, if an S-system admits a Lie transformation group, an equation can be decoupled by introduction of new variables  $\xi_i = X_i X_n^{-\nu_i/\nu_n}$  as shown above (cf. Eq. (2.9)), and the resulting system is in multinomial form. In fact, the invariants  $\xi_i$  that are used in this transformation have exactly the same structure as the auxiliary variables that are introduced in the reduction of multinomial systems to the S-system form.

### References

- Chen, C.-T., Linear System Theory and Design, Holt, Rinehart and Winston, Inc., New York 1984
- [2] Irvine, D.H., Savageau, M.A., Numerical solution of nonlinear ordinary differential equations expressed in canonical forms, SIAM J. Num. Anal. 27 (1990), 704–735
- Janszen, D.B., PB-PK: An Interactive Physiologically-Based Pharmacokinetic Modeling and Simulation System, Ph.D. Dissertation, Medical University of South Carolina 1992
- [4] Kokotovic, P.V., O'Malley, Jr., R.E., Sannuti, P., Singular perturbations and order reduction in control theory - An overview, Automatica 12 (1976), 123–132
- [5] Savageau, M.A., Growth equations: a general equation and a survey of special cases, Math. Biosci. 48 (1980), 267–278
- [6] Savageau, M.A., Voit, E.O., Recasting nonlinear differential equations as S-systems: A canonical nonlinear form, Math. Biosci. 87 (1987), 83-115
- [7] Thompson, J.M.T., Stewart, H.B., Nonlinear Dynamics and Chaos, J. Wiley and Sons, Chichester 1986
- [8] Troch, I., Müller, P.C., Fasol, K.H., Modellreduktion für Simulation and Reglerentwurf. Autommatisierungstechnik (1992: in press)
- [9] Voit, E.O. (ed.), Canonical Nonlinear Modeling: S-System Approach to Understanding Complexity, Van Nostrand Reinhold, New York 1991
- [10] Voit, E.O., Symmetries of S-systems, Math. Biosci. 109 (1992), 19-37
- [11] Voit, E.O., Rust, P.F., Tutorial: S-system analysis of continuous univariate probability distributions, J. Stat. Comput. Simul. 42 (1992), 187–249
- [12] Wright, R., The information age, The Sciences (July/Aug. 1987), 2–5