Lotka–Volterra Representation of General Nonlinear Systems

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ABSTRACT

In this article we elaborate on the structure of the generalized Lotka–Volterra (GLV) form for nonlinear differential equations. We discuss here the algebraic properties of the GLV family, such as the invariance under quasimonomial transformations and the underlying structure of classes of equivalence. Each class possesses a unique representative under the classical quadratic Lotka–Volterra form. We show how other standard modeling forms of biological interest, such as S-systems or mass-action systems, are naturally embedded into the GLV form, which thus provides a formal framework for their comparison and for the establishment of transformation rules. We also focus on the issue of recasting of general nonlinear systems into the GLV format. We present a procedure for doing so and point at possible sources of ambiguity that could make the resulting Lotka–Volterra system dependent on the path followed. We then provide some general theorems that define the operational and algorithmic framework in which this is not the case. © *Elsevier Science Inc., 1997*

1. INTRODUCTION

The search and study of canonical representations (reference formats that are form invariant under a given set of transformations) in nonlinear systems of ordinary differential equations has been a recurrent theme in the literature. Although the powerful algebraic structure that characterizes the theory of linear differential systems does not seem to have a counterpart in the nonlinear realm (a not so surprising fact, once we take into consideration the apparent diversity in structure and richness of behaviors of nonlinear vector fields), there is an increasing

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number of suggestions for a partial solution to this problem, which we partly review later in this article.

Recasting an n-dimensional differential system into a canonical form conveys a gain in algebraic order that is not without cost, for it has usually to be embedded in a higher-dimensional mathematical structure. The procedure is then justified if in the context of the target canonical form we are in possession of powerful mathematical tools allowing for a better analysis of the original system. This is not always the case, for not all suggested canonical forms provide, in this sense, a satisfactory level.

The Lotka–Volterra structure can be considered one of the favored forms to this effect. First, it may qualify for canonical form in a classical context, for Plank [1] has demonstrated that n-dimensional Lotka–Volterra equations are Hamiltonian and are thereby amenable to a classical canonical description once an appropriate Poisson structure is chosen. Second, its paramount importance in ecological modeling equals its ubiquity in all fields of science, from plasma physics [2] to neural nets [3]. This may not be unrelated to the fact that it is quadratic, and thus appears in many models in which interaction processes are viewed as fortuitous "collisions," or "encounters," between at most two constitutive entities, those with more than two participants being seen as extremely improbable. Additionally, it is characterized by simple algebraic objects as matrices, which makes its analysis far more attractive than that of other formats. Also, being representable in terms of a network, it spans a bridge to a possible connection to a graph theory approach in the qualitative study of nonlinear differential equations, either directly or through its equivalence with the well-known replicator equations [4].

The purpose of this article is to elaborate on the algebraic structure of the so-called generalized Lotka–Volterra (GLV) formalism, defined on equations the structure of which generalizes the n-dimensional Lotka–Volterra system—it contains them as a particular case. It thus offers a natural bridge toward the representation of nonlinear systems in terms of Lotka–Volterra equations. We also review other known canonical forms, paying special attention, due to its biological implications, to the so-called S-system format, introduced by Savageau and co-workers as a potential way to approach nonlinear systems [5, Chap. 1]. We show how the GLV formalism offers a formal solution to the issue of transformations between different canonical forms, a problem that has already attracted the attention of Voit and Savageau in the case involving Lotka–Volterra and S-system forms [6].

Despite the versatility of the GLV equations, they do not seem *at first sight* to encompass many model systems of biological or physical

significance, with, for example, saturating rates defined in terms of
rational functions. This exclusion is, however, only apparent, for it is a
well-known fact that nonpolynomial rate laws are always amenable to a
polynomial format by the introduction of conveniently chosen auxiliary
variables. This trick, which was known from old in the field of celestial
mechanics [7], was popularized by Kerner [8] and independently by
Savageau and collaborators [5, Chap. 12], who have made ample use of
this technique. Although the GLV equations are somewhat different
from polynomial ones, there is no obstacle for applying the same
procedure, as we show. The problem is that the above technique is
unfortunately not systematic, as it relies on a clever selection of the
additional variables and of their derivatives (as we see later) and does
not generally lead to a unique system in any one of the desired formats,
let it be polynomial, S-system, or any other whatsoever (in our case in
GLV form). This ambiguity, and the resulting multiplicity of target
systems (an infinite number is not so uncommon), may throw some
shadow on the procedure and may be especially confusing when a single
choice of auxiliary variables leads to the disclosure of several entirely
different target systems or, reversely, when a single target system
originates from completely different choices of auxiliary variables.

No doubt, the previous method of auxiliary variables has important
drawbacks, but it is presently the only known course of action when
confronted with this type of recasting problem. The limits of these
ambiguities should be then clearly outlined, for it is essential to en-
hance the confidence in the applicability of the method. This task is
carried out in the final sections of the article.

2. OVERVIEW OF CANONICAL FORMS

A. Infinite-dimensional linear systems: If the theory of linear vector
fields has been given a well-defined and coherent structure, can we
somehow linearize? This sensible question was given an answer in 1931
by T. Carleman [9], following Poincaré's suggestion. He showed that a
finite-dimensional system of ordinary polynomial differential equations
is equivalent to an infinite-dimensional linear system of ODEs. The
whole issue lay dormant until the late seventies. Since then, several
authors have greatly contributed to the investigation of the potential
applications of the Carleman embedding, which have been recently
reviewed by Kowalski and Steeb [10]. Although there has been an
interesting suggestion of a "quantum mechanical" formalism applicable
to the Carleman linearization, the scheme does not seem to provide, for
the time being, an operationally acceptable framework. Additionally,

the manipulation of an infinite-dimensional system, as linear as it may be, can still be considered objectable by many users.

B. Riccati systems: Some time ago Kerner [8] proposed a scheme with the purpose of bringing general nonlinear differential systems down to polynomial vector fields and ultimately to what he termed *elemental Riccati systems*:

$$\dot{x}_i = \sum_{j,k} A_i^{jk} x_j x_k,$$

with A_i^{jk} either 0 or 1. He suggests doing so by introducing step-by-step new variables that represent collectives of other variables and by making use of the sequential differentiation rule—in a way similar to that of the Carleman embedding. This rather heuristic recipe is the traditional, and widely used, method for reducing the degree of a nonlinearity. The dimension of the elemental Riccati system is, of course, greater than that of the initial system; but the gain in structure—that is, in order—is not without cost.

C. Mass action systems: Chemical kinetics has been considered by certain authors a good candidate for prototype in nonlinear science [11]. They claim that it would already deserve this consideration if it were only because it embraces all types of behavior of interest, from multiplicity of steady states to chaotic evolution, with the backing of a large *corpus* of experimental evidence. The simplicity of the stoichiometric rules and that of the algebraic structure of the corresponding evolution equations has made chemical kinetics a traditional point of reference in modeling within fields such as population biology [12], quantitative sociology [13], prebiotic evolution [4], and other biomathematic problems [14], where a system is viewed as a collection of "species" interacting as molecules do. As emphasized by Erdi and Tóth [11], even the algebraic structure of the evolution equations from many other fields can be converted into "chemical language," where a formal "analog" in terms of a chemical reaction network is defined. However, the serious obstacle of negative cross effects was emphasized by Tóth and Hárs [15], by showing that no orthogonal transformation leads the Lorenz and Rössler systems to a "kinetic" format. Although many suggestions have been made to overcome the difficulty of the negative cross effects [16–19], the problem seems to remain unsolved.

D. S-systems: S-systems constitute an interesting canonical form that has been developed in the context of the power-law formalism in theoretical biochemistry. Its proponents have made a considerable effort in showing how it is a good candidate for representing general nonlinear systems, as well as in elaborating on its relation to other forms, from generalized mass action to Lotka–Volterra systems [5,

Chap. 12]. Its particularly simple form

$$\dot{x}_i = \alpha_i \prod_{j=1}^{n} x_j^{g_{ij}} - \beta_i \prod_{j=1}^{n} x_j^{h_{ij}}, \qquad i = 1, \ldots, n,$$

optimal estimation of parameter values from steady-state experiments and the possibility of symbolic steady-state analysis [5, Chap. 6] have been proposed, among others, as arguments to justify the choice of S-systems. Although some preliminary steps have been covered [5, Chap. 15; 20], much work is still necessary to provide the S-systems formalism with a proper formal framework yielding a workable algebraic structure, wherefrom insight on their mathematical properties might be gained. We pay special attention to S-systems in the present article. We do it by showing how they find their place within the generalized Lotka–Volterra formalism.

   E. Lotka–Volterra systems: The well-known n-dimensional Lotka–Volterra (LV) equations,

$$\dot{x}_i = \lambda_i x_i + x_i \sum_{j=1}^{n} A_{ij} x_j, \qquad i = 1, \ldots, n, \qquad (1)$$

have obvious quadratic nonlinearities and are characterized by simple algebraic objects: matrices λ and A. Although they have occupied a privileged position in ecology—practically all high dimensional *strategic* models are set in terms of them—they also appear in many other fields, such as virology, where the concept of *quasispecies* has given a whole new perspective [21,22]. Cairó and Feix [23] refer to a fairly long list of systems modeled by LV equations, a sample that speaks in favor of their representative role and has prompted Peschel and Mende [24] to give their book on the issue the title: *Do we Live in a Volterra World?* We may also recall that Lotka–Volterra equations are also equivalent to game dynamical equations, replicator, or autocatalytic networks [4]. Through this connection, LV dynamics is linked to the whole fruitful field of replicator dynamics and autocatalytic networks, which is a continuous source of modeling in prebiotic evolution, game dynamics, or population genetics. LV systems are given a privileged status in what is to follow.

3. GENERALIZED LOTKA–VOLTERRA FORMALISM

   The term *generalized Lotka–Volterra equations* has been recently coined by Brenig [25] to refer to a system of the form

$$\dot{x}_i = \lambda_i x_i + x_i \sum_{j=1}^{m} A_{ij} \prod_{k=1}^{n} x_k^{B_{jk}}, \qquad i = 1, \ldots, n, \qquad (2)$$

where m is a positive integer not necessarily equal to n. Following Brenig [25], vectors x and λ and the $n \times m$ matrix A and $m \times n$ matrix B may be indifferently real or complex. However, we assume in what follows that the x_i are real and positive and that the matrix entries are arbitrary real numbers. The importance of (2) as a representation of Lotka–Volterra models was previously studied by Peschel and Mende [24, p. 120 ff], who anticipated many of the interesting properties of the algebraic structure of (2) (they termed them *multinomial differential systems*). These equations also appear in independent developments by Br'uno [26] and Gouzé [27]. They embrace a large category of relevant systems of differential equations and can be considered as equivalent to the generalized mass-action systems (GMA), which have been dealt with by Savageau and co-workers [5].

Several important properties reveal the potential interest of the GLV equations (2). We may start by recalling some propositions from Peschel and Mende [24, Sect. 5.2], Brenig and Goriely [28], and Hernández-Bermejo and Fairén [29], which we summarize in a single theorem:

THEOREM 1

(i) *GLV equations (2) are form invariant under quasimonomial power transformations*:

$$x_i = \prod_{k=1}^{n} y_k^{C_{ik}}, \qquad i = 1, \ldots, n, \tag{3}$$

defined by any nonsingular (in our case, real) $n \times n$ matrix, C. In other words, the system of equations obtained from Eqs. (2) by a quasimonomial transformation (3) is also a GLV system of the same dimension. Moreover, if we denote such a system as

$$\dot{y}_i = \hat{\lambda}_i y_i + y_i \sum_{j=1}^{m} \hat{A}_{ij} \prod_{k=1}^{n} y_k^{\hat{B}_{jk}}, \qquad i = 1, \ldots, n, \tag{4}$$

then

$$\hat{\lambda} = C^{-1} \cdot \lambda, \qquad \hat{A} = C^{-1} \cdot A, \qquad \hat{B} = B \cdot C. \tag{5}$$

(ii) *The product matrices,*

$$\hat{B} \cdot \hat{\lambda} = B \cdot \lambda, \qquad \hat{B} \cdot \hat{A} = B \cdot A, \tag{6}$$

are invariants under the quasimonomial transformations (3). The whole family of systems (2) is then split into classes of equivalence according to relations (6), such that, for given values of n and m, to each class of

equivalence specific realizations of the product matrices $B \cdot \lambda$ and $B \cdot A$ can be associated.

(iii) *The quasimonomials*

$$\prod_{k=1}^{n} x_k^{B_{jk}}, \qquad j = 1, \ldots, m, \tag{7}$$

constitute a set of m invariants of the class of equivalence to which the corresponding GLV system belongs.

(iv) *All GLV systems* (2) *defined in an open subset of the positive orthant that belong to the same class of equivalence are topologically equivalent; that is, their phase spaces can be mapped into each other by a diffeomorphism* [30], *given by* (3).

In particular, the importance of quasimonomial transformations in what follows cannot be underestimated. Their relevance has been clearly emphasized in the literature (see [24, Sects. 5.2 and 5.4] and [25, 26]). These transformations have also been used by Voit to study symmetry properties of GMA systems in [5, Chap. 15] and [20].

3.1. THE LOTKA–VOLTERRA CANONICAL FORM

To go further ahead in detailing the features of the GLV formalism in the context of its canonical forms we should now distinguish three independent cases, two of which have been studied by Brenig and Goriely ($m = n$, $m > n$) while the third ($m < n$) is considered in here for the first time. We find it necessary to elaborate on them all, for they will help us in understanding the recasting technique, which we use for embedding S-systems into the GLV formalism.

3.1.1. Case $m = n$

A and B in (2) are $n \times n$ square matrices. We consider some specific transformation matrices C, which lead to interesting canonical forms. Assume first that B is invertible and C is taken as B^{-1}. According to (5), $\hat{B}$ reduces to the identity matrix and (4) takes the usual LV form,

$$\dot{y}_i = \hat{\lambda}_i y_i + y_i \sum_{j=1}^{n} \hat{A}_{ij} y_j, \qquad i = 1, \ldots, n. \tag{8}$$

By construction, for those classes of equivalence with nonsingular matrices B there is a unique LV representative. It is interesting to observe that, according to (3), each of the variables y_j in (8) is actually

$$y_j = \prod_{k=1}^{n} x_k^{B_{jk}}, \qquad j = 1, \ldots, n. \tag{9}$$

In other words, each of the variables in the LV scheme (8) accounts for one of the different nonlinear quasimonomials in (2).

3.1.2. *Example with $m = n$*

We reduce to the Lotka–Volterra canonical form the generic GLV system:

$$\dot{x}_1 = x_1 [\lambda_1 + a_{11} x_1^p + a_{12} x_2^q]$$

$$\dot{x}_2 = x_2 [\lambda_2 + a_{21} x_1^p + a_{22} x_2^q].$$

If we perform a transformation of the form (3) with matrix $C = B^{-1}$, we are led to a LV system with matrices $\hat{A} = B \cdot A$ and $\hat{\lambda} = B \cdot \lambda$. It is

$$\dot{y}_1 = y_1 [p\lambda_1 + p a_{11} y_1 + p a_{12} y_2]$$

$$\dot{y}_2 = y_2 [q\lambda_2 + q a_{21} y_1 + q a_{22} y_2],$$

where $y_1 = x_1^p$ and $y_2 = x_2^q$.

3.1.3. *Case $m > n$*

Here, the number of quasimonomials m is higher than that of independent variables. Accordingly, the target LV form (8) is to be an m-dimensional system, its variables standing for the m quasimonomials in (2). The transformation of Section 3.1.1 cannot be carried out unless (2) is previously embedded in an equivalent m-dimensional system. To do so we enlarge system (2) by introducing $m - n$ auxiliary "arguments," to which we assign a fixed value, $x_l = 1$, $l = n + 1, \ldots, m$ and that enter the equations like

$$\dot{x}_i = \lambda_i x_i + x_i \sum_{j=1}^{m} A_{ij} \prod_{k=1}^{n} x_k^{B_{jk}} \left[x_{n+1}^{B_{j,n+1}} \ldots x_m^{B_{jm}} \right], \qquad i = 1, \ldots, n, \quad (10)$$

with arbitrary values of $B_{j,n+1}, \ldots, B_{jm}$: We are in fact adding $m - n$ arbitrary columns to the $m \times n$ matrix B to complete a nonsingular $m \times m$ matrix $\tilde{B}$. In (10), the term in brackets should not affect the equations as long as the new arguments stick to their assigned value. We do ensure it by defining for them the equations

$$\dot{x}_l = \lambda_l x_l + x_l \sum_{j=1}^{m} A_{lj} \prod_{k=1}^{n} x_k^{B_{jk}} \left[x_{n+1}^{B_{j,n+1}} \ldots x_m^{B_{jm}} \right], \qquad l = n + 1, \ldots, m,$$

$$(11)$$

with entries $\lambda_l = 0$ and $A_{lj} = 0$, for $l = n+1,\ldots,m$, and initial conditions, $x_l(0) = 1$. Then, (10) and (11) define an expanded m-dimensional system to which the procedure of Section 3.1.1 can be applied. This embedding technique preserves the topological equivalence between the initial and final systems, as has been demonstrated in [29].

3.1.4. *Example with $m > n$*

As an example, we consider a simple spheroid model for tumor growth, due to Marušić et al. [31]:

$$\dot{V} = V[-3\omega + 3\alpha k^{1/3}V^{-1/3} - 3\alpha k^{2/3}V^{-2/3} + \alpha kV^{-1}], \qquad \alpha, k, \omega > 0.$$

Here V denotes the tumor volume, provided $V \geq k$. We perform the embedding described by Equations (10) and (11). The matrices of the expanded system are given by

$$\tilde{A} = \begin{pmatrix} 3\alpha k^{1/3} & -3\alpha k^{2/3} & \alpha k \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}; \qquad \tilde{B} = \begin{pmatrix} -1/3 & 0 & 0 \\ -2/3 & 1 & 0 \\ -1 & 0 & 1 \end{pmatrix};$$

$$\tilde{\lambda} = \begin{pmatrix} -3\omega \\ 0 \\ 0 \end{pmatrix}.$$

We are now in the case $n = m$. The resulting LV system is thus

$$\dot{y}_1 = y_1[\omega + \mu_1 y_1 + \mu_2 y_2 + \mu_3 y_3]$$
$$\dot{y}_2 = y_2[2\omega + 2\mu_1 y_1 + 2\mu_2 y_2 + 2\mu_3 y_3]$$
$$\dot{y}_3 = y_3[3\omega + 3\mu_1 y_1 + 3\mu_2 y_2 + 3\mu_3 y_3],$$

where $\mu_1 = -\alpha k^{1/3}$, $\mu_2 = \alpha k^{2/3}$, and $\mu_3 = -\alpha k/3$.

3.1.5. *Case $m < n$*

In this case, the number of quasimonomials, m, is smaller than that of variables, n. Consequently, there is no need to perform an embedding, as in the previous case. Only m variables of the n-dimensional LV system will stand for the m original quasimonomials, while the $n - m$ remaining variables of that same LV system, as we shall see, will have an arbitrary dependence on the original variables. This means, as we can guess, that only m variables are actually independent. In fact, we demand that the $m \times n$ $\hat{B}$ matrix of the target LV system be of the form $\hat{B} = (I_{m \times m} \mid 0_{m \times (n-m)})$ (save row and column permutations), where I is

the identity matrix, 0 is the null matrix, and the subindexes indicate the sizes of these submatrices. On the other hand, we also have from (5) that $\hat{B} = B \cdot C$. If Z denotes the inverse of matrix C, we have $\hat{B} \cdot Z = B$. Since the structure of $\hat{B}$ is very simple, we can explicitly evaluate, and write

$$B = \begin{pmatrix} z_{11} & \cdots & z_{1n} \\ \vdots & \ddots & \vdots \\ z_{m1} & \cdots & z_{mn} \end{pmatrix}. \tag{12}$$

Thus, the first m rows of $Z = C^{-1}$ are given by the entries of matrix B from the original GLV system. Since C must be an invertible matrix, we have demonstrated the following result:

THEOREM 2

   If $m < n$, a necessary and sufficient condition for the existence of a transformation (3) leading to a LV system is that matrix B is of rank m.

The procedure continues straightforwardly by completing the $n - m$ undefined rows of Z with arbitrary selected entries, which make the resulting matrix invertible. There are infinite ways of doing this, generating a multiplicity of LV systems present in the corresponding class of equivalence. If $m = n$, we would obtain directly $Z = B$: a known result from Section 3.1.1. In other words, all features of the limit case $n = m$ are preserved when $m < n$, with the only exception being the uniqueness of the LV system: Now we have infinite LV systems in a given class of equivalence.

3.1.6.   *Example with $m < n$*

   We consider the following GLV system:

$$\dot{x}_1 = x_1\left(-1 + x_1 x_2 x_3 + x_1^2 x_2 x_3^2\right) \tag{13}$$

$$\dot{x}_2 = x_2\left(3 + 2x_1 x_2 x_3 + x_1^2 x_2 x_3^2\right) \tag{14}$$

$$\dot{x}_3 = x_3\left(2 - x_1 x_2 x_3 + 2x_1^2 x_2 x_3^2\right). \tag{15}$$

We choose the LV matrix B of the form (the row permutation is irrelevant)

$$\hat{B} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}.$$

Consequently:

$$\begin{pmatrix} z_{21} & z_{22} & z_{23} \\ z_{11} & z_{12} & z_{13} \end{pmatrix} = B = \begin{pmatrix} 1 & 1 & 1 \\ 2 & 1 & 2 \end{pmatrix}.$$

We now complete Z with an arbitrary third row: (1 0 0) for example. Then $C = Z^{-1}$. After evaluation of C, $\hat{A}$ and $\hat{\lambda}$ can be obtained, and the resulting LV system is:

$$\dot{y}_1 = y_1(5 + 7y_1 + 2y_2)$$

$$\dot{y}_2 = y_2(4 + 4y_1 + 2y_2)$$

$$\dot{y}_3 = y_3(-1 + y_1 + y_2),$$

where $y_1 = x_1^2 x_2 x_3^2$ and $y_2 = x_1 x_2 x_3$, and stand for the two quasimonomials present in (13)–(15). As mentioned above, the $n - m$ remaining variables (here y_3) have been freely chosen, a fact that implies the selection of one of the infinite existing LV systems in the class of equivalence. We should nevertheless note that the m actually independent variables (here y_1 and y_2) obey a unique Lotka–Volterra system. As far as this is valid we can also claim in this case the uniqueness of the Lotka–Volterra as representative of a class of equivalence.

3.2. SINGLE-QUASIMONOMIAL CANONICAL FORM

We briefly mention another form that proves to be of interest in later sections [24, p. 124].

3.2.1. Case $m = n$

For any class of equivalence for which A is nonsingular we can choose $C = A$. In this case we have for (4),

$$\dot{y}_i = \hat{\lambda}_i y_i + y_i \prod_{k=1}^{n} y_k^{\hat{B}_{ik}}, \qquad i = 1, \dots, n. \tag{16}$$

This canonical form has interesting integrability properties, which have been studied in depth by Goriely and Brenig [32].

On the other hand, it is clear that if all λ's are nonpositive, Equation (16) is also an S-system. We find this similarity useful and consider in a forthcoming section an example of the single quasimonomial canonical form under the viewpoint of the S-system recasting technique.

3.2.2. *Case m > n*

As in Section 3.1.3, a preliminary embedding of the original GLV equation in an m-dimensional system is also a prescriptive requirement prior to the application of the procedure for case $m = n$ and the achievement of this canonical form. However, this time the embedding must be such that the extended matrix A be invertible. To satisfy this condition, Brenig and Goriely [28] introduce $m - n$ auxiliary variables such that

$$\dot{x}_\alpha = \begin{cases} \lambda_\alpha x_\alpha + x_\alpha \sum_{\beta=1}^{m} A_{\alpha\beta} \prod_{\gamma=1}^{n} x_\gamma^{B_{\beta\gamma}} \left[x_{n+1}^0 \cdots x_m^0 \right], & \alpha = 1,\ldots,n \\ \rho_\alpha x_\alpha + x_\alpha \sum_{\beta=1}^{m} a_{\alpha\beta} \prod_{\gamma=1}^{n} x_\gamma^{B_{\beta\gamma}} \left[x_{n+1}^0 \cdots x_m^0 \right], & \alpha = n+1,\ldots,m. \end{cases}$$

We can then proceed as in Section 3.2.1. A proof, which is rather involved, of the topological invariance of the solutions under this embedding process will be provided in a future work.

4. S-SYSTEMS WITHIN THE GLV FORMALISM

The observation that a generic S-system

$$\dot{x}_i = \alpha_i \prod_{j=1}^{n} x_j^{g_{ij}} - \beta_i \prod_{j=1}^{n} x_j^{h_{ij}}, \qquad i = 1,\ldots,n,$$

is in fact a particular case of GLV system allows us to focus attention on applying the previous formalism to the inverse problem, that is, the conversion of a GLV system into an equivalent S-system. We see how the recasting procedure can now be standardized within the formalism we have presented. We complement the multiple heuristic recipes quoted for this purpose [5, Chap. 12] by presenting a formal strategy that allows a nonnegligible freedom of design of target S-system matrices, within the obvious restriction of topological equivalence (TE). This TE will be ensured if the target S-system is reachable through any element of the infinite group of quasimonomial transformations. This and the ability to predict the dimension, number, and exact definition of the variables are some of the advantages derived from dealing with the problem in a well-characterized mathematical framework.

We again study the problem of recasting into S-systems in three steps of increasing complexity:

4.1. *CASE m = n*

4.1.1. *Recasting Theory*

We start from a GLV system

$$\dot{x}_i = x_i \left(\lambda_i + \sum_{j=1}^{n} A_{ij} \prod_{k=1}^{n} x_k^{B_{jk}} \right), \qquad i = 1\ldots n. \tag{17}$$

We must apply a quasimonomial transformation to (17) and proceed consequently to a new GLV system (with matrices $\hat{\lambda}, \hat{A}, \hat{B}$) *to which we also demand the fulfillment of an S-system format specifications*. This target system must be designed while taking into account the fact that, according to the S-system form, in every equation there is only one positive and one negative term (the linear term is also a possible term in an S-system). To find the right transformation matrix, C, we rewrite Equations (5) by introducing the *extended matrices* E and D, associated to the GLV system (17) and to the transformation matrix C respectively:

$$E = \begin{pmatrix} 1 & \mathbf{0}^t \\ \lambda & A \end{pmatrix}, \qquad D = \begin{pmatrix} 1 & \mathbf{0}^t \\ \mathbf{0} & C \end{pmatrix}, \qquad \{E, D\} \subset \mathscr{M}_{(n+1) \times (n+1)}. \quad (18)$$

Then the GLV system matrices A, B, and λ are equivalently specified by E and B. The equivalence between C and D is obvious. When a transformation of the kind (3) is performed, the GLV matrices change to:

$$\hat{B} = B \cdot C, \qquad \hat{E} = D^{-1} \cdot E. \quad (19)$$

By means of this construction, which is very useful later, the following result can be easily demonstrated:

THEOREM 3

   Suppose that $m = n$ and that matrices A and λ of system (17) possess arbitrary real entries. Assume the target S-system is characterized by some specifically chosen matrices $\hat{\lambda}$ and $\hat{A}$. Then, there exists a unique transformation of the form (3), given by $C = A \cdot \hat{A}^{-1}$, which leads from (17) to such an S-system, provided matrices A and $\hat{A}$ are regular and vectors λ and $\hat{\lambda}$ can be related by the compatibility condition $\lambda = A \cdot \hat{A}^{-1} \cdot \hat{\lambda}$.

   Note also that in the general case the design of the final S-system can be done easily by working directly with the extended matrix $\hat{E}$. That is, the rule is that every row of $\hat{E}$ must contain only two nonzero elements, one of which is positive and the other negative.
   On the other hand, the compatibility condition of Theorem 3 yields a system of equations with n^2 unknown quantities (the entries of matrix $C = A \cdot \hat{A}^{-1}$). The application of the Rouché–Fröbenius theorem [33] shows there there will always be infinite solutions to such a system, thus ensuring precisely the fulfillment of that same compatibility condition.
   As we can see, there exist infinite different S-systems in every class of equivalence. In the case $n = m$, however, there is a single LV system,

provided matrix B is regular: the one resulting through the election $C = B^{-1}$. In fact, it is straightforward to note that in this case such an LV system can be chosen as the canonical element of the class.

A remarkable feature of the previous theory is the complete freedom in the choice of the form for matrix $\hat{A}$. This means that the last theorem can be applied equally to any kind of canonical form, not necessarily that of an S-system. For example, choosing a diagonal matrix $\hat{A}$ we construct a family of systems that includes the single quasimonomial canonical form as a special case [25, 28]. As we see subsequently, this freedom is maintained in the other general situations.

4.1.2. *Example with m = n*

We recast the system of Section 3.1.2 as an S-system. The original system is characterized by the two matrices:

$$B = \begin{pmatrix} p & 0 \\ 0 & q \end{pmatrix}, \qquad E = \begin{pmatrix} 1 & 0 & 0 \\ \lambda_1 & a_{11} & a_{12} \\ \lambda_2 & a_{21} & a_{22} \end{pmatrix}.$$

We may wish to transform our starting system into, for example, an S-system defined by matrix:

$$\hat{E} = \begin{pmatrix} 1 & 0 & 0 \\ \mu_1 & -\sigma_1 & 0 \\ \mu_2 & 0 & -\sigma_2 \end{pmatrix}, \qquad \mu_i, \sigma_i > 0, \; i = 1, 2.$$

According to the prescription of Theorem 3 we assume that $|A| = a_{11}a_{22} - a_{12}a_{21} \neq 0$. Additionally, the compatibility condition implies that

$$\begin{pmatrix} \mu_1 / \sigma_1 \\ \mu_2 / \sigma_2 \end{pmatrix} = -A^{-1} \begin{pmatrix} \lambda_1 \\ \lambda_2 \end{pmatrix} \equiv \begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix}.$$

The quantities ξ_1 and ξ_2 must be positive in order to have a consistent set of equations. If this is the case we may then set, for example, $\sigma_i = 1$ and $\mu_i = \xi_i$, $i = 1, 2$. Note that $\hat{A} = -I$ with this choice of parameters. We infer, from Theorem 3, $C = A \cdot \hat{A}^{-1} = -A$. Consequently, our new variables are

$$y_1 = x_1^{-\Delta a_{22}} x_2^{\Delta a_{12}}$$

$$y_2 = x_1^{\Delta a_{21}} x_2^{-\Delta a_{11}},$$

where $\Delta = (|A|)^{-1}$. We thereby obtain a matrix B of the form

$$\hat{B} = B \cdot C = - \begin{pmatrix} pa_{11} & pa_{12} \\ qa_{21} & qa_{22} \end{pmatrix},$$

the target S-system being given by

$$\dot{y}_1 = \xi_1 y_1 - y_1^{1+pa_{11}} y_2^{pa_{12}}$$
$$\dot{y}_2 = \xi_2 y_2 - y_1^{qa_{21}} y_2^{1+qa_{22}}.$$

4.2. CASE $m > n$
4.2.1. Recasting theory

The general solution of this problem requires the introduction of one or more auxiliary new variables: In fact, without the aid of an embedding the recasting of a GLV system into an S-system may be rigorously impossible in some cases, as the following theorem shows:

THEOREM 4

If $m > 2n$ there exists no quasimonomial transformation (3), *which leads from a GLV system to an equivalent S-system.*

In systems not precluded by Theorem 4, a unified description shall proceed by reducing to the $m = n$ case through the same embedding technique of Section 3.2.2. The advantage of this particular embedding is that it leads to an expanded GLV system whose matrix $\tilde{A}$ is regular and allows the direct application of Theorem 3. We skip a formal description and go directly to illustrate the matter with an example.

4.2.2. Example with $m > n$

We recast as an S-system the tumor growth model of Section 3.1.4. Once embedded, we can follow the procedure of the $m = n$ case. We write the corresponding extended matrices of the embedded system

$$\tilde{E} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 3\omega & 3\alpha k^{1/3} & -3\alpha k^{2/3} & \alpha k \\ -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix}; \qquad \tilde{B} = \begin{pmatrix} -1/3 & 0 & 0 \\ -2/3 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix},$$

where, for convenience, we have expanded the original vector $\lambda = (3\omega)$ with two elements of value -1. We now investigate the recasting of this GLV system as a target S-system of extended matrix:

$$\hat{E} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ -a' & a & 0 & 0 \\ -b' & 0 & b & 0 \\ -c' & 0 & 0 & c \end{pmatrix}.$$

All constants are taken as strictly positive. We look once more for the fulfillment of the compatibility condition of Theorem 3, which leads us to the matrix identity:

$$
\begin{pmatrix} 3\omega \\ -1 \\ -1 \end{pmatrix} = \begin{pmatrix} -3\alpha k^{1/3}a'/a + 3\alpha k^{2/3}b'/b - \alpha k c'/c \\ -b'/b \\ -c'/c \end{pmatrix}.
$$

We may choose, for example, the values for our parameters,

$$
a = b = c = b' = c' = 1; \qquad a' = \gamma, \; \gamma = k^{1/3} - \tfrac{1}{3}k^{2/3} - \alpha^{-1}\omega k^{-1/3},
$$

which yields for our target S-system the extended matrix,

$$
\hat{E} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ -\gamma & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix}.
$$

It is worth noting how all the complexity of the system has been conveyed into a single constant, γ. Also, from Theorem 3, the transformation matrix is given by $C = \tilde{A} \cdot \hat{A}^{-1} = \tilde{A}$. Since $\hat{A} = I$, our target system is also, by definition, the single quasimonomial canonical form. Solving for $\hat{B} = \tilde{B} \cdot C = \tilde{B} \cdot \tilde{A}$ we obtain that the final system of equations is

$$
\dot{y}_1 = -\gamma y_1 + y_1^{1+\mu_1} y_2^{\mu_2} y_3^{\mu_3}
$$

$$
\dot{y}_2 = -y_2 + y_1^{2\mu_1} y_2^{1+2\mu_2} y_3^{2\mu_3}
$$

$$
\dot{y}_3 = -y_3 + y_1^{3\mu_1} y_2^{3\mu_2} y_3^{1+3\mu_3},
$$

where the μ's are defined as in the example of Section 3.1.4. This system, which coincides with the single quasimonomial canonical form, will be also an S-system provided that the values of the constants k, α and ω are such that γ is positive or zero. Since $C = \tilde{A}$, the value of V can be now straightforwardly retrieved as $V = y_1^{-3\mu_1} y_2^{-3\mu_2} y_3^{-3\mu_3}$.

4.3. CASE $m < n$

4.3.1. Recasting Theory

Once again, the situation here is formally similar to the one where $m = n$, the only differences arising from the fact that here the extended matrices E and $\hat{E}$ are not square. This means that, once $\hat{E}$ has been

designed, the equation to solve is $D \cdot \hat{E} = E$, where D must comply to format (18). The existence and uniqueness of D will depend on the ranks of the matrices involved.

4.3.2. Example with $m < n$

We here analyze the example of 3.1.6. We choose the following S-system extended matrix,

$$\hat{E} = \begin{pmatrix} 1 & 0 & 0 \\ 1 & -1 & 0 \\ 0 & 2 & -1 \\ 0 & 1 & 0 \end{pmatrix}.$$

Then we are led to the following matrix equation:

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & c_{11} & c_{12} & c_{13} \\ 0 & c_{21} & c_{22} & c_{23} \\ 0 & c_{31} & c_{32} & c_{33} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 1 & -1 & 0 \\ 0 & 2 & -1 \\ 0 & 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ -1 & 1 & 1 \\ 3 & 2 & 1 \\ 2 & -1 & 2 \end{pmatrix}.$$

In this example there exists a unique solution, given by

$$C = \begin{pmatrix} -1 & -1 & 2 \\ 3 & -1 & 7 \\ 2 & -2 & 5 \end{pmatrix}.$$

Solving for $\hat{B}$ we reach the following target S-system:

$$\dot{y}_1 = y_1 - y_1^5 y_2^{-4} y_3^{14}$$

$$\dot{y}_2 = 2 y_1^4 y_2^{-3} y_3^{14} - y_1^5 y_2^{-6} y_3^{21}$$

$$\dot{y}_3 = y_1^4 y_2^{-4} y_3^{15}.$$

5. GENERAL NONLINEAR SYSTEMS WITHIN THE GLV FORMALISM

5.1. THE AUXILIARY VARIABLES PROCEDURE

To briefly describe the auxiliary variable method that we have mentioned earlier, we proceed by a very general approach. We may start by assuming that we have at hand an n-dimensional system dependent on what we can define to be a set of r functions, $\{f_k\}$, which

do not comply with the quasimonomial form, given by (2). We elaborate on a system that has previously rearranged into the form

$$\dot{x}_i = x_i \left(\lambda_i + \sum_{j=1}^{m} A_{ij} \prod_{k=1}^{n} x_k^{B_{jk}} \prod_{s=1}^{r} f_s^{C_{js}} \right), \qquad i = 1, \ldots, n, \qquad (20)$$

which is a GLV-like form except for the set $\{f_k\}$. Our concern is to examine the circumstances in which (20) can be rewritten as a GLV system.

For this purpose, we take into account that most of the functions that are actually used in modeling in a biological context (elementary, most of them) obey equations relating their partial derivatives to members of the properly chosen set $\{f_k\}$ itself in the following way:

$$\frac{\partial f_k}{\partial x_i} = \sum_{r=1}^{m'} E_r^{(ik)} \prod_{j=1}^{n} x_j^{G_{rj}^{(ik)}} \prod_{s=1}^{r} f_s^{H_{rs}^{(ik)}} \qquad i = 1, \ldots, n, \ k = 1, \ldots, r. \quad (21)$$

The set $\{f_k\}$ must be appropriately defined to fulfill (21). If, for example, the circular sine-function appears in (20), the cosine-function will correspondingly be present in (21). The set then includes both functions, the cosine-function appearing with an exponent zero in (20).

Thus, if the set $\{f_k\}$ has been appropriately defined, that is, such that (20) and (21) hold, it is then straightforward to obtain a GLV form by assigning each function f_k to an extra variable y_k and taking into consideration that

$$\dot{y}_k = \sum_{i=1}^{n} \frac{\partial f_k}{\partial x_i} \dot{x}_i. \qquad (22)$$

5.2. SOURCES OF AMBIGUITY

So far, everything seems consistent to the procedure developed in 5.1. However, there is some degree of arbitrariness as far as equations (20)–(22) are ambiguously defined. We point to two sources of ambiguity:

1. The set of functions $\{f_k\}$ is certainly not unique. Any other set $\{F_i\}$, such as

$$F_i = \left(\prod_{k=1}^{r} f_k^{q_{ik}} \right) \left(\prod_{j=1}^{n} x_j^{p_{kj}} \right), \qquad i = 1, \ldots, r', \qquad (23)$$

will also comply with the general starting prescribed forms (20) and (21). This statement holds in all three cases: $r < r'$; $r = r'$; $r > r'$.

2. Any chosen set of functions $\{f_k\}$ may be compatible with more than one expression for each of its partial derivatives (21), and thus generate different GLV systems.

We see that there is a substantial difference between the two previous propositions. While the issue raised in point 1 is shown to be formally cleared and settled in three subsequent general theorems, that forwarded in point 2 cannot conversely be given a general formal foothold and has to rely on a rather empirical knowledge from a collection of examples; let it be infinite. This difference will result in a consistent solution to the problem posed by the ambiguity of point 1; a task we undertake in the present article. On the contrary, the problem set in point 2 cannot be formally solved, although we later comment on its consequences.

We now state three theorems in connection to point 1:

THEOREM 5

Let $\{f_k\}$ and $\{F_k\}$ be two sets of a number r of C^1-functions defined on the strictly positive orthant of $\Re^n$, which we denote int $\Re_+^n$. For every k, we assume $f_k > 0$ and $F_k > 0$ for all $x \in$ int $\Re_+^n$.
   Then, if

$$F_i = \left(\prod_{j=1}^{r} f_j^{q_{ij}} \right) \left(\prod_{k=1}^{n} x_k^{p_{ik}} \right), \tag{24}$$

we have

   i. *The inverse transformation from the set $\{F_k\}$ to the set $\{f_k\}$ is defined iff* $\det Q \neq 0$, with $(Q)_{ij} = q_{ij}$, $i, j = 1, \ldots, r$.
   ii. *The transformations defined by (24) constitute a parametric group,* $\Xi \equiv \{\xi(Q, P)\}$, where $(P)_{ik} = p_{ik}$, $k = 1, \ldots, n$.

THEOREM 6

Let $r = \text{card}\{f_k\}$ and $r' = \text{card}\{F_i\}$ in (23). Suppose $r \neq r'$ and $\rho = \max\{r, r'\}$. Let Q be an $r' \times r$ matrix defined as in Theorem 5. If $\text{rank}(Q)$ is maximum, there exists two new sets of ρ functions, in which $\{f_k\}$ and $\{F_i\}$ can be embedded, and for which the statement of Theorem 5 holds.

THEOREM 7

Equations (20) and (21) are form invariant under the group Ξ.

The set whose elements are themselves those sets of functions generated through the action of the group Ξ on the set $\{f_k\}$ constitute a class of equivalence $\Gamma\{f_k\}$. According to the procedure of Section 5.1,

each member of a class Γ will be mapped onto a GLV system, which will eventually differ from that obtained by applying the same procedure to any other element of the class. The question is to know if, in spite of that, all elements of a class Γ are mapped into a single GLV class of equivalence. We answer it in Sections 5.3 and 6.

5.3. HEURISTIC CONSIDERATIONS ON AN ILLUSTRATIVE MODEL SYSTEM

Before supplying the reader with the formal theorems that demonstrate that the class of equivalence $\Gamma\{f_k\}$, generated by the group of transformations Ξ, is mapped into a single GLV class of equivalence by applying the procedure of Section 5.1, we make a heuristic analysis of a simple one-dimensional model. It was introduced by Ludwig et al. [34] to simulate the evolution of the population of the spruce budworm in the presence of predation by birds. In dimensionless form it is

$$\dot{x} = rx\left(1 - \frac{x}{k}\right) - \frac{x^2}{1 + x^2}. \tag{25}$$

Let us thus consider the model system defined by (25). To recast it into the GLV format we can initially choose the following function $f = (1 + x^2)^{-1}$ with derivative $f'(x) = -2xf^2$. According to the casuistry of the previous section we examine what happens for a general transform $y = F = x^p f^q$, $q \neq 0$. After elementary calculations, we obtain from (25):

$$\dot{x} = x\left[r - \frac{r}{k}x - x^{1-p/q}y^{1/q}\right]$$

$$\dot{y} = y\left[pr - \frac{pr}{k}x - px^{1-p/q}y^{1/q}\right.$$

$$\left. - 2rqx^{2-p/q}y^{1/q} + \frac{2rq}{k}x^{3-p/q}y^{1/q} + 2qx^{3-2p/q}y^{2/q}\right]. \tag{26}$$

It is straightforward to check that the products $B \cdot A$ and $B \cdot \lambda$ are independent of exponents p and q. That means that all parameter-dependent GLV systems (26) do actually belong to a single GLV class of equivalence and makes the result of the procedure independent of any specific choice of auxiliary variables within the class of functions $x^p f^q$. Thus, the class $\Gamma\{f\}$ is mapped into a single GLV class of equivalence. We generalize this assertion for any function in Section 6.

The previous invariance is not so surprising. In fact, (24) and the functions $x^p f^q$ are disguised forms of quasimonomial transformations [25], and these map into one another different GLV systems within a

given GLV class of equivalence, leaving $B \cdot A$ and $B \cdot \lambda$ invariant. The quasimonomials of the GLV systems are also invariants of the class [29]. In the present case, from (26):

$$x; x^{1-p/q} y^{1/q} = x/(1+x^2);$$
$$x^{2-p/q} y^{1/q} = x^2/(1+x^2);$$
$$x^{3-p/q} y^{1/q} = x^3/(1+x^2);$$
$$x^{3-2p/q} y^{2/q} = x^3/(1+x^2)^2.$$

We now examine the context of Theorem 6. For that we may start from two different sets of functions to deal with the problem, for example,

$$\{f_1\} = \left\{\frac{1}{1+x^2}\right\}, \qquad \{F_1, F_2\} = \left\{\frac{1}{1+x^2}, \frac{x^3}{1+x^2}\right\}.$$

According to Theorem 6, set $\{f_1\}$ is embedded into set $\{f_1, f_2\}$, with $f_2 \equiv 1$. Then both sets, $\{f_k\}$ and $\{F_k\}$, are related through an invertible transformation of form (5) with matrices

$$Q = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}, \qquad P = \begin{pmatrix} 0 \\ 3 \end{pmatrix}.$$

Note that the second column of matrix Q is arbitrary: The only requirement imposed by Theorem 6 is that Q must be invertible. If we use the set $\{f_1, f_2\}$ to carry out the substitution in (25), we arrive at the following system:

$$\dot{x} = x\left[r - \frac{r}{k}x - xy_1\right]$$
$$\dot{y}_1 = y_1\left[-2rx^2 y_1 + \frac{2r}{k}x^3 y_1 + 2x^3 y_1^2\right] \qquad (27)$$
$$\dot{y}_2 = 0.$$

If, on the contrary, we start from $\{F_1, F_2\}$, we are led to the system

$$\dot{x} = x\left[r - \frac{r}{k}x - xy_1\right]$$
$$\dot{y}_1 = y_1\left[-2rx^2 y_1 + \frac{2r}{k}y_2 + 2x^3 y_1^2\right] \qquad (28)$$
$$\dot{y}_2 = y_2\left[3r - \frac{3r}{k}x - 3xy_1 - 2rx^2 y_1 + \frac{2r}{k}y_2 + 2x^3 y_1^2\right].$$

It can be easily checked that, after the apparently naive introduction of the function $f_2 = 1$, systems (27) and (28) belong to the same class of equivalence: Both possess the same quasimonomials and the same matrix invariants $B \cdot A$ and $B \cdot \lambda$.

We can, however, skip the application of Theorem 6 and introduce both sets of auxiliary functions independently, namely $\{f_1\}$ and $\{F_1, F_2\}$. In this case the result is the same as before, with the only difference that the last equation in system (27) does not exist now. Consequently, the two systems cannot be in a same class of equivalence, since the number of variables is different in each case. Nevertheless it can be easily seen that the quasimonomials and the matrix invariants still coincide. As a consequence, we can make use of a general procedure we have seen in Section 3.1.3 for the reduction of these GLV systems to a common class of equivalence: the Lotka−Volterra embedding. When we perform such an embedding over both systems, the result will be GLV systems with five variables and five quasimonomials, both in the same class of equivalence. In particular, the systems are equivalent to a 5×5 Lotka−Volterra system of matrices $\tilde{A} = B \cdot A$ and $\tilde{\lambda} = B \cdot \lambda$. We can thus infer that, independently of the number of auxiliary variables of form $x^p f^q$ that we introduce in system (25), once the definitions of f and its derivative are fixed, all the (p, q)-dependent GLV systems we obtain can be embedded into the same class of equivalence.

We conclude the section by examining what happens when we start from different forms of the derivative. If, for example, we set

$$f = \frac{x^2}{1 + x^2},\qquad(29)$$

there are in fact infinite possible definitions of the derivative for this function, namely:

$$\frac{df}{dx} = 2x^{-2n-3} f^{n+2} (1 + x^2)^n, \qquad n = 0, 1, 2 \ldots.$$

It can be easily checked that, in general, different expressions of the derivative lead to different quasimonomials, both in number and form, and consequently to different classes of equivalence (point (iii) of Theorem 1).

6. EMBEDDING INTO THE GLV FORM

We now proceed to formalize the results obtained in Section 5.3. There is no conceptual objection in dealing with a single nonquasimonomial function f. This is what we do from now on to develop the

essential features of the problem with the greatest simplicity. We thus consider a system of the general form:

$$\dot{x}_s = \sum_{i_{s1},\ldots,i_{sn},j_s} a_{i_{s1}\cdots i_{sn}j_s} x_1^{i_{s1}} \cdots x_n^{i_{sn}} f(\bar{x})^{j_s}$$

$$x_s(t_0) = x_s^0, \qquad s = 1,\ldots,n. \tag{30}$$

We additionally assume that $f(\bar{x})$ is such that its partial derivatives can be expressed in the form

$$\frac{\partial f}{\partial x_s} = \sum_{e_{s1},\ldots,e_{sn},e_s} b_{e_{s1}\cdots e_{sn}e_s} x_1^{e_{s1}} \cdots x_n^{e_{sn}} f(\bar{x})^{e_s}. \tag{31}$$

All constants in (30) and (31) are assumed to be real numbers.

The procedure to transform (30) and (31) into a GLV system is then straightforward. We know from Section 5 that this can be carried out by introducing a set of l additional variables of the form

$$y_r = f^{q_r} \prod_{s=1}^{n} x_s^{p_{rs}}, \qquad q_r \neq 0, \forall r = 1 \cdots l, \tag{32}$$

with real exponents q_r, p_{rs}. For the time being, we assume that a given value of l is selected; that is, we deal with a fixed number of auxiliary variables. We later release this requirement.

The introduction of the auxiliary variables (32) leads to the following system for the original variables:

$$\dot{x}_s = x_s \left[\sum_{i_{s1},\ldots,i_{sn},j_s} a_{i_{s1}\cdots i_{sn}j_s} y_1^{j_s/q_1} \prod_{k=1}^{n} x_k^{i_{sk}-\delta_{sk}-j_s p_{1k}/q_1} \right] \tag{33}$$

for $s = 1,\ldots,n$. As usual, $\delta_{sk} = 1$ if $s = k$, and 0 otherwise. For the new variables (32) we obtain

$$\dot{y}_r = \sum_{s=1}^{n} \frac{\partial y_r}{\partial x_s} \dot{x}_s = y_r \left[\sum_{s=1}^{n} \left\{ p_{rs} x_s^{-1} \dot{x}_s \right. \right.$$

$$\left. \left. + \sum_{i_{s\alpha},j_s,e_{s\alpha},e_s} a_{i_{s\alpha},j_s} b_{e_{s\alpha}e_s} q_r y_r^{(e_s+j_s-1)/q_r} \prod_{k=1}^{n} x_k^{i_{sk}+e_{sk}+(1-e_s-j_s)p_{rk}/q_r} \right\} \right], \tag{34}$$

where $\alpha = 1,\ldots,n$. Appropriate initial conditions $y_r(0)$ must also be included (this is assumed whenever a new variable is introduced). Thus, with (33) and (34) the reduction of system (30) to the GLV format is

achieved. Note that, from (32), the expression of f in terms of the y_r is not unique. It has been specified, in (33), in terms of y_1, but this could have been done by choosing any other variable y_r. We prove that this choice is irrelevant.

Let us now focus attention on the generic GLV system (33)–(34). It is clear that different systems are obtained for distinct choices of the auxiliary variables (32). We first demonstrate that all these systems are part of one and the same equivalence class [25, 29], that is:

THEOREM 8

Let us assume a specific realization for Equations (30) *and* (31). *Then, all GLV systems — Eqs.* (33)–(34) — *generated by the introduction of a given number l of auxiliary variables* (32) *belong to the same class of equivalence.*

All systems complying with the format (33)–(34) are in the same GLV class of equivalence: According to the previous results they must thus possess identical quasimonomials. This can be easily checked if we rewrite such quasimonomials in terms of the original variables $\bar{x}$ and $f(\bar{x})$. The corresponding equations for the x_s are

$$\dot{x}_s = x_s \left[\sum_{i_{s1},\ldots,i_{sn},J_s} a_{i_{s1}\cdots i_{sn}J_s} f^{J_s} \prod_{k=1}^{n} x_k^{i_{sk} - \delta_{sk}} \right] \tag{35}$$

with $s = 1,\ldots,n$. For the y_r we obtain

$$\dot{y}_r = y_r \left[\sum_{s=1}^{n} \left\{ p_{rs} x_s^{-1} \dot{x}_s + \sum_{i_{s\alpha}J_s e_{s\alpha} e_s} a_{i_{s\alpha}J_s} b_{e_{s\alpha} e_s} q_r f^{e_s + J_s - 1} \prod_{k=1}^{n} x_k^{i_{sk} + e_{sk}} \right\} \right], \tag{36}$$

where $\alpha = 1,\ldots,n$. The quasimonomials, as functions of x_k, $k = 1,\ldots,n$, do not depend in any way on the definition of the auxiliary variables (32), but only on constants from (30)–(31).

We can then state the following proposition:

COROLLARY 9

For a given number l of auxiliary variables, the GLV class of equivalence in which (30) *is embedded is completely determined by the choices for $f(\bar{x})$ and the particular representation of its derivatives* (31).

Irrespectively of the number l of auxiliary variables, we have classes of equivalence with the same m quasimonomials. Moreover, in all these classes the matrix invariants $B \cdot A$ and $B \cdot \lambda$ are of sizes $m \times m$ and

$m \times 1$, respectively. This makes us suspect that those products can also be identical, as in the case of the quasimonomials. This would imply that, after an appropriate embedding (see Section 3.1.3), we could include all those systems into the same class of equivalence of m-dimensional systems, independently of the actual value of l. The next theorem shows that this is the case.

THEOREM 10

Let us assume, as in Theorem 8, a specific realization for Eqs. (30) and (31). Let us consider the set Φ of all $(n + l)$-dimensional systems (33)–(34), obtained from all possible choices of auxiliary variables (32), as l varies in the interval $1 \le l \le m - n$, where m is the number of quasimonomials. Then, all elements of Φ can be embedded in a single GLV class of equivalence of m-dimensional systems.

Thus it has been demonstrated that, independently of the number l, $1 \le l \le (m - n)$ and specific form of variables of type (32), the final class obtained is always the same, since the m invariant quasimonomials and the matrices $B \cdot A$ and $B \cdot \lambda$ are completely independent of those degrees of freedom. We also have the following:

COROLLARY 11

All elements of the set Φ can be embedded in a unique m-dimensional Lotka–Volterra system.

7. DIRECT CALCULATION OF THE QUASIMONOMIALS

An important issue in the practical application of Theorem 10 and Corollary 11 is that of the knowledge of the m quasimonomials, which are actually going to be the variables of the target m-dimensional Lotka–Volterra system. These quasimonomials can be evaluated directly from Equations (30)–(31), without any need to first comply with the GLV form (33)–(34).

An important previous definition is that of *vector of exponents* associated with a given quasimonomial $x_1^{i_1} \cdots x_n^{i_n} f(\bar{x})^j$. The vector of exponents is a shorthand notation in which this quasimonomial is expressed as $(i_1, \ldots, i_n \mid j)$. Since the order of the variables is implicit in this "vector," all the information about the quasimonomial is contained in it.

Thus the algorithm consists of the following sequential rules:

1. Build the vectors of exponents for all the quasimonomials present in both Equations (30) and (31). We label such sets of vectors E_s for the sth equation in (30):

$$E_s = \{(i_{s1}, \ldots, i_{sn} \mid j_s)\},$$

and D_s for the sth equation in (31):

$$D_s = \{(e_{s1},\ldots,e_{sn} \mid e_s)\}.$$

Note that these families of vectors must be constructed separately for both Eqs. (30) and (31).

2. In the $\dot{x}_s$ equation of the GLV system the quasimonomials will be

$$\{(i_{s1},\ldots,i_{ss} - 1,\ldots,i_{sn} \mid j_s)\}.$$

This expression is obviously to be applied over all vectors in E_s.

3. While in the $\dot{y}_r$ GLV equation:

• Those quasimonomials already present in $\dot{x}_s$, for all $s = 1,\ldots,n$, such that $p_{rs} \neq 0$.

• Those coming from all pairwise combinations of elements of E_s and D_s, such that:

$$(i_{s1} + e_{s1},\ldots,i_{sn} + e_{sn} \mid j_s + e_s - 1),$$

for all $s = 1,\ldots,n$.

This constructive evaluation also makes straightforward the derivation of algebraic expressions for bounds to the number m of quasimonomials, or, equivalently, upper and lower bounds to the phase-space dimension of the target class, as we have:

THEOREM 12

If $\varepsilon_s = \operatorname{card}(E_s)$ and $\delta_s = \operatorname{card}(D_s)$:
• An upper bound to m is:

$$\omega = \sum_{s=1}^{n} (1 + \delta_s)\varepsilon_s$$

• A lower bound to m is:

$$\alpha = \operatorname{card}\left\{ \bigcup_{s=1}^{n} [E_s \backslash (\delta_{s1},\ldots,\delta_{sn} \mid 0)] \right\} + \delta_{1n},$$

where $\delta_{\alpha\beta}$ is Kronecker's delta.

We can observe that, the shorter the expressions for the derivatives, the smaller the upper bound. This establishes an economy principle in election (31).

To illustrate the preceding results, we can make use of the example of Section 5.3:

$$\dot{x} = rx\left(1 - \frac{x}{k}\right) - \frac{x^2}{1 + x^2},$$

$$f = \frac{1}{1 + x^2}, \qquad \frac{df}{dx} = -2xf^2.$$

We evaluate the quasimonomials resulting from the introduction of a generic auxiliary variable of the form $y = x^p f^q$, $q \neq 0$. The sets of vectors are $E_1 = \{(1 \mid 0), (2 \mid 0), (2 \mid 1)\}$, and $D_1 = \{(1 \mid 2)\}$. We thus have $\varepsilon = 3$ and $\delta = 1$. Since $\text{card}\{E_1 \backslash (1 \mid 0)\} = 2$ and $n = 1$, the bounds to the number of quasimonomials are $\alpha = 3$ and $\omega = 6$.

By applying the second rule, we see that the quasimonomials in the $\dot{x}$ equation are: $(0 \mid 0)$, which is a constant and must be discarded; $(1 \mid 0) = x$ and $(1 \mid 1) = xf$. From the third rule, if $p \neq 0$, the set $\{x, xf\}$ will also be present in the $\dot{y}$ equation. This equation will always contain the quasi-monomials $(2 \mid 1) = x^2 f$, $(3 \mid 1) = x^3 f$, and $(3 \mid 2) = x^3 f^2$. Thus, we find five different quasimonomials. The confirmation that they coincide with those in the explicit system (26) is straightforward (see Section 5.3).

8. FINAL COMMENTS

The structure of the generalized Lotka–Volterra equations has been shown to provide an ideal setting for codifying in a unified framework the relations between different formats of practical use when modeling in terms of ordinary differential equations.

When encapsulated in the context of the GLV formalism, a given model finds itself embedded in a class of equivalence, the members of which define an infinite set of models topologically equivalent to one another. It is found that a class of equivalence may contain several members belonging to those representative canonical forms we men-tioned before, each one of them being mapped into another by the quasimonomial transformation rules, but a single LV representative. For these reasons, together with the Hamiltonian properties of the Lotka–Volterra equations [1], this form may rightly deserve to be called *canonical*.

Finally, if the GLV formalism is to be of any practical use, in addition to its algebraic structure it must comply to the requirement of providing a framework for the fairly general class of model systems whose vector field either does not obey its format or cannot be rewrit-ten in some trivial way in terms of it. We have demonstrated that this is possible. The way in which this can be unambiguously done has been the issue of the concluding sections of the work.

APPENDIX

We carry out those demonstrations of previous theorems that are nontrivial.

Proof of Theorem 8.   Given two different choices of auxiliary variables

$$y_r = f^{q_r} \prod_{s=1}^{n} x_s^{p_{rs}},\ y_r' = f^{q_r'} \prod_{s=1}^{n} x_s^{p_{rs}'},\ r = 1,\ldots,l; \qquad q_r, q_r' \neq 0\ \forall r,$$

the resulting sets of GLV variables will be, respectively, $(x_1,\ldots,x_n, y_1,\ldots,y_l) \equiv (x_1,\ldots,x_{n+l})$ and $(x_1,\ldots,x_n, y_1',\ldots,y_l') \equiv (\hat{x}_1,\ldots,\hat{x}_{n+l})$. An easy calculation shows that both sets of variables are connected through a quasimonomial transformation of the kind

$$x_i = \prod_{k=1}^{n+l} \hat{x}_k^{C_{ik}}, \qquad i = 1,\ldots,n+l,$$

with C given by

$$C = \begin{pmatrix} I_{n \times n} & O_{n \times l} \\ \tilde{A}_{l \times n} & \tilde{B}_{l \times l} \end{pmatrix},$$

where the dimension of the submatrices is indicated by the subindexes, I is the identity matrix, O is the zero matrix, $\tilde{A}_{ij} = \alpha_{ij}$, $\tilde{B}_{ij} = \beta_i \delta_{ij}$, with

$$\alpha_{rs} = p_{rs} - \beta_r p_{rs}', \qquad \beta_r = \frac{q_r}{q_r'}.$$

Consequently, both systems are members of the same class.   ∎

Proof of Theorem 10.   We shall write for simplicity the GLV system (33)–(34) in the equivalent form

$$\dot{x}_i = x_i \left(\lambda_i + \sum_{j=1}^{m} A_{ij} \prod_{k=1}^{n+l} x_k^{B_{jk}} \right), \qquad i = 1,\ldots,n+l,\ m \geq n+l.$$

When we perform the changes (32) for different numbers of new variables, that is, for different values of l, we arrive at different-sized GLV systems. However, for a given l all of them lead to the same Lotka–Volterra system, since they belong to the same GLV class of

equivalence. Moreover, from (33)–(34) we know that all of them possess the same quasimonomials (the Lotka–Volterra variables) independently of l. Thus, in order to complete this proof, we only need to demonstrate that the Lotka–Volterra matrices $B' = B \cdot A$ and $\lambda' = B \cdot \lambda$ do not depend on l, either. We can do this by induction.

First, we consider the case $l = 1$. If we introduce a single new variable $y_1 = x_{n+1}$ of the kind (32), the GLV system will be characterized by three matrices A, B, λ. If we add to this system a second auxiliary variable $x_{n+2} = y_2$, a simple way to write the corresponding $m \times (n+2)$ matrix $\tilde{B}$ is

$$\tilde{B} = (B, 0),$$

where the 0 indicates that the last column of $\tilde{B}$ is composed of zeros. We denote as $\tilde{A}$ and $\tilde{\lambda}$ the other two matrices of this system for which $l = 2$. Note that $\mathrm{rank}(\tilde{B}) = n + 1$, so this matrix is not of maximal rank and cannot be employed to perform an embedding of the kind showed in Section 3.1.3. Nevertheless, this does not affect this demonstration, since we consider all possible matrices, including those of maximal rank, starting from this one: Suppose that we reexpress the quasimonomials as powers of the variables $x_1, \ldots, x_n, x_{n+1}, x_{n+2}$, but with a choice of the exponents different to the one given by $\tilde{B}$. These exponents will be the entries of a new matrix $\tilde{B}'$ (there are infinite possibilities for this alternative description). The equality of the ith quasimonomial, $1 \leq i \leq m$, implies

$$x_1^{b_{i,1}} x_2^{b_{i,2}} \cdots x_{n+1}^{b_{i,n+1}} = x_1^{b'_{i,1}} \cdots x_n^{b'_{i,n}} x_{n+1}^{b'_{i,n+1}} x_{n+2}^{b'_{i,n+2}}, \tag{37}$$

where b, b' are the elements of $\tilde{B}, \tilde{B}'$ respectively. It is important to note that x_{n+2} is not independent of the rest of the variables $x_1, \ldots, x_n, x_{n+1}$:

$$x_{n+2} = x_{n+1}^{\alpha} \prod_{k=1}^{n} x_k^{\beta_k}, \qquad \alpha \neq 0.$$

If we substitute this expression into (37) and regroup in the left side we are led to

$$\left(\prod_{j=1}^{n} x_j^{b_{i,j} - b'_{i,j} - \beta_j b'_{i,n+2}} \right) x_{n+1}^{b_{i,n+1} - b'_{i,n+1} - \alpha b'_{i,n+2}} = 1. \tag{38}$$

Since all the variables in (38) are independent, the only solution is that the exponents are identically zero. We can rewrite this condition as

$$\tilde{B}' = \tilde{B} - Q,$$

with

$$(Q)_{ij} = \begin{cases} b'_{i,n+2}\,\beta_j, & 1 \le j \le n \\ b'_{i,n+2}\,\alpha, & j = n+1 \\ -b'_{i,n+2}, & j = n+2. \end{cases}$$

The relationships among the coefficients of the quasimonomials in (33)–(34) imply the vanishing of the products $Q \cdot \tilde{A}$ and $Q \cdot \tilde{\lambda}$. This step of the proof involves simple but lengthy algebra. We do not detail it. Then, $\tilde{B}' \cdot \tilde{A} = \tilde{B} \cdot \tilde{A}$, and $\tilde{B}' \cdot \tilde{\lambda} = \tilde{B} \cdot \tilde{\lambda}$, and the theorem is proved for the case $l = 2$.

In a similar way it can be shown that this equality holds for the step $l \to l+1$ in the induction procedure. Again the algebra is simple but the process is tedious and is not reproduced here.   ■

Proof of Theorem 12.   The lower bound in the case $n \ne 1$ and the upper bound are obvious consequences of rules 2 and 3 of the algorithm. The demonstration then reduces to prove that if $n = 1$

$$\omega = \text{card}\{E_1 \backslash (1\,|\,0)\} + 1.$$

To understand the addition of 1 to this expression we need a previous lemma:

LEMMA

If $n = 1$ there exists $(\alpha\,|\,\beta) \in D_1$ such that $(\alpha\,|\,\beta) \ne (-1\,|\,1)$.

Proof of the Lemma.   Suppose that the lemma is false: Then $D_1 = \{(-1\,|\,1)\}$. Consequently

$$\frac{df}{dx} = kx^{-1}f$$

and f is of the form cx^k with c a real constant. This contradicts the assumption of a nonquasipolynomial f and demonstrates the lemma.

We return to the theorem. Taking into account the fact stated in this lemma, the proof for the case $n = 1$ holds by a simple counting procedure: If $D_1 = \{(-1\,|\,1)\}$, then rule 3 of the algorithm automatically repeats the quasimonomials generated from rule 2, all of them of the form $(i-1\,|\,j)$. However, since $D_1 \ne \{(-1\,|\,1)\}$, at least one new quasimonomial will appear from rule 3, which is not generated by rule 2.   ■

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