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Algebraic recasting of nonlinear systems of ODEs into universal formats

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Abstract. It is sometimes desirable to produce for a nonlinear system of ODEs a new representation of simpler structural form, but it is well known that this goal may imply an increase in the dimension of the system. This is what happens if in this new representation the vector field has a lower degree of nonlinearity or a smaller number of nonlinear contributions. Until now both issues have been treated separately, rather unsystematically and, in some cases, at the expense of an excessive increase in the number of dimensions. We unify here the treatment of both issues in a common algebraic framework. This allows us to proceed algorithmically in terms of simple matrix operations.

1. Introduction

We are frequently interested in transforming a given system of nonlinear ODEs into some specified format. Some of these formats are, given their very simple structure, particularly attractive. One is the generalized Riccati format—or the Lotka–Volterra equations, as one of its variants. There are many other useful formats such as the generalized mass action, used in modelling chemical reactions or in metabolic control theory [1]; S-systems, devised to capture the saturable characteristics of nonlinear systems [1]; the unimonomial canonical form [2], which has proved to be suitable for analysing integrability properties; etc.

Reformatting a system of ODEs finds its more rewarding field of application in the obtainment of approximate solutions, especially numerical. It is in the field of celestial mechanics where this approach was first systematically carried out [3], by rewriting equations of motion into polynomial form and expanding solutions in terms of a Taylor-like integration scheme. This procedure has been shown to lead to time-saving and highly accurate integrators [4, 5], specifically adapted to symbolic manipulation [6]. Irvine *et al* [7] also argued in favour of reformatting before proceeding to a numerical integration. Actually, additional constants of motion introduced in some recasting procedures may prove useful for exploiting certain families of numerical algorithms used in symplectic or Poisson formulations [8]. By preserving exactly first integrals we may indirectly measure the accuracy of the numerical approximation.

Loosely speaking, two will essentially be the ultimate goals of reformatting procedures: (i) an equivalent system of lower degree of nonlinearity—quadratic at most, for example;

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(ii) or alternatively, a vector field with a smaller number of contributions—terms—in its components. Generally, the system must be embedded into some higher-dimensional set of equations in order to be recasted into the target format. This happens if the manipulation aims at a reduction in the degree of the nonlinearity defining the vector field. Examples are: the Carleman embedding [9, 10], where an n -dimensional system of nonlinear ODEs is set into the form of an infinite-dimensional linear system, or Kerner's procedure [11] for reducing nonlinearities to quadratic form.

Resorting to an embedding may also be the case if we wish instead to reduce the number of nonlinear terms building up the components of the vector field. This is necessary in the study of certain integrability properties of ODEs in parameter space [2]. Also, in some modelling approaches in theoretical biochemistry [12, 13], where net rates of variation in concentration of species are split into the sum of a single inflow and outflow terms. Finally, in the case of half-systems and binary half-systems [12], rates are reduced to a single contribution per equation.

The problem with the different procedures used nowadays in recasting is that they are rather unsystematic, relying too much on a rule of thumb approach to the problem. In this paper we wish to treat the issue from a systematic point of view. We choose as an appropriate framework to do so a format for the vector field defined in terms of quasipolynomial expressions, which has proven to be suitable for representing general nonlinear vector fields [13, 14]. It has been indifferently called generalized Lotka–Volterra format [2], generalized mass action systems [12], multinomial differential systems [15], power-law rates systems [16] and polynomial differential systems [17]. The distinctive property of the quasipolynomial format is that it is form-invariant under certain classes of transformations, called quasimonomial and new-time transformations. Consequently, its analysis can be carried out in terms of simple matrix algebra.

This paper is organized as follows. In sections 2.1 and 2.2 we outline the basic algebraic properties of systems of quasipolynomial ODEs, which will define our operational framework. In sections 2.3–2.5 we demonstrate how an arbitrary quasipolynomial system can be reduced to a standard form which will constitute the starting point in later sections. Sections 3 and 4 are the core of this work: we explain and illustrate the reduction procedure for the degree of nonlinearity and number of nonlinear terms, respectively. We give some concluding remarks in section 5.

2. The quasipolynomial formalism

We shall consider a quasipolynomial (QP) system of ODEs of the form [18]

$$\dot{x}_i = x_i \left(\lambda_i + \sum_{j=1}^m A_{ij} \prod_{k=1}^n x_k^{B_{jk}} \right) \quad i = 1 \dots n \quad (1)$$

where n and m are positive integers, and A , B and λ are $n \times m$, $m \times n$ and $n \times 1$ real matrices, respectively. Sometimes it will also be convenient to consider the $n \times (m + 1)$ composed matrix $M = (\lambda|A)$. We shall also assume that the x_i are real and positive (if this is not the case, an appropriate phase-space translation is to be performed on the variables in order to ensure positiveness, see [14]). In what follows, n will always denote the number of variables of a QP system, and m the number of the quasimonomials

$$\prod_{k=1}^n x_k^{B_{jk}} \quad j = 1 \dots m. \quad (2)$$

2.1. Dimension-preserving transformations

System (1) is formally invariant under quasimonomial transformations [2]

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

for any invertible real matrix C . Under (3), matrices B, A, λ and M change to

$$B' = B \cdot C \quad A' = C^{-1} \cdot A \quad \lambda' = C^{-1} \cdot \lambda \quad M' = C^{-1} \cdot M \tag{4}$$

respectively, but the QP format is preserved. An (n, m) -family of QP systems is thus split into classes of equivalence, the product $B \cdot M$ being a class invariant. Under the previous assumptions, the solutions of all the members of the class are topologically equivalent [14].

The quasimonomial transformations are complemented by new-time transformations of the form [19, 20]

$$dt = \left(\prod_{i=1}^n x_i^{\beta_i} \right) dt' \tag{5}$$

where the β_i are real constants. Equation (5) also preserves the QP format.

2.2. Transformations that do not preserve dimension

A QP system can be subjected to some interesting additional manipulations that do not preserve the actual dimension.

We may, on the one hand, embed a system (1) into a larger QP system by means of an expansion of matrices B and M up to any arbitrary p

$$B \longrightarrow \tilde{B} = (B|B_{m \times p}) \quad M \longrightarrow \tilde{M} = \begin{pmatrix} M \\ O_{p \times (m+1)} \end{pmatrix} \tag{6}$$

with arbitrary entries for matrix $B_{m \times p}$. Here, $O_{p \times (m+1)}$ is the $p \times (m + 1)$ null matrix. By this embedding we add p new variables which remain constant under the action of the expanded vector field (6), for all $t \geq 0$. The original equations are not altered if the initial values for these p additional variables are chosen to be equal to one.

On the other hand, another transformation can be defined as

$$B \longrightarrow \tilde{B} = (B|O_{m \times p}) \quad M \longrightarrow \tilde{M} = \begin{pmatrix} M \\ M_{p \times (m+1)} \end{pmatrix}. \tag{7}$$

The entries of $M_{p \times (m+1)}$ are in principle arbitrary. By this operation we simply add to the original system (1) p variables in such a way that in the expanded system the original n variables are not coupled to these p new variables.

Without loss of generality, we shall assume in forthcoming sections that the QP system under study has $m \geq n$, and that the ranks of matrices A and B are both maximal (i.e. $\text{rank}(A) = \text{rank}(B) = n$). In what remains of the section we proceed to demonstrate for the first time that any QP system not fulfilling these requirements can be reduced to this standard situation.

The algorithm proceeds in three steps.

(1) Reduction to the case $m \geq n$, by means of a quasimonomial transformation which reduces the solution for some of the variables to a quadrature.

(2) When $m \geq n$, reduction to a system with maximal rank of B . The method is similar to that in (1).

- (3) When $m \geq n$ and $\text{rank}(B)$ is maximal, reduction to a system with maximal rank of A . There are two steps:
- (3.1) reduction to maximal rank of M by means of a quasimonomial transformation, followed by the decoupling of some variables;
 - (3.2) reduction to maximal rank of A by means of a new-time transformation.

2.3. Reduction to the case $m \geq n$

Assume a QP system for which $m < n$. Let $\text{rank}(B) = r$, with $r \leq m$. Since B is an $m \times n$ matrix, $\dim\{\ker(B)\} = (n - r) > 0$. Consequently, we can perform a quasimonomial transformation of matrix

$$C = \left(\begin{array}{c|c} I_r & \\ \hline O_{(n-r) \times r} & \phi^{(r+1)} \dots \phi^{(n)} \end{array} \right) \quad (8)$$

where I_r is the $r \times r$ identity matrix, and $\{\phi^{(r+1)}, \dots, \phi^{(n)}\}$ is a set of column vectors which constitute a basis of $\ker(B)$. When applied, the quasimonomial transformation given by matrix (8) leads to $B' = (B'_{m \times r} | O_{m \times (n-r)})$. This implies that we are led to an r -dimensional QP system for x_1, \dots, x_r , plus $(n - r)$ quadratures for x_{r+1}, \dots, x_n . The problem is thus reduced to the case $m \geq n$ (with $n = r$).

2.4. Reduction to a system with maximal rank of B

Let us assume now a QP system with $m \geq n$, and $\text{rank}(B)$ not maximal. As Brenig and Gorieli [19] have shown, the system can be transformed into an equivalent one for which $\text{rank}(B)$ is maximal. The technique is similar to that in section 2.3: if $r = \text{rank}(B)$, $r < n$, then $(n - r)$ variables can be decoupled by means of transformation (8). The result now is a QP system of r variables and m quasimonomials plus $(n - r)$ quadratures.

2.5. Reduction to a system with maximal rank of A

Here we shall proceed in two steps. First, we shall demonstrate how a QP system can be reduced to an equivalent one for which $\text{rank}(M)$ is maximal. Then, the scope of the result shall be enlarged to the reduction to a system with maximal rank of A . As before, we assume $m \geq n$.

We solve the first part of the problem by giving two new constructive theorems.

Theorem 1. If $\text{rank}(M) = r < n$ in equations (1), then there exist $(n - r)$ time-independent first integrals of the system. Moreover, these first integrals are functionally independent, and thus the system evolves on a manifold of dimension r .

Proof. We can assume, without loss of generality, that the r first rows of M are linearly independent. Then, there exist real constants γ_{ki} , $1 \leq i \leq r$, $r + 1 \leq k \leq n$, such that:

$$M_{kl} = \sum_{i=1}^r \gamma_{ki} M_{il} \quad 1 \leq l \leq m + 1. \quad (9)$$

From the form of equations (1), this implies:

$$\frac{\dot{x}_k}{x_k} = \sum_{i=1}^r \gamma_{ki} \frac{\dot{x}_i}{x_i}. \quad (10)$$

After a simple integration this leads to the set of $(n - r)$ first integrals:

$$x_k^{-1} \prod_{i=1}^r x_i^{\gamma_{ki}} = c_k \tag{11}$$

where the c_k are real constants given by the initial conditions. Their functional independence is ensured if the rank of the corresponding Jacobian F is maximal. It is straightforward to see that as $\text{rank}(F) = (n - r)$, the $(n - r)$ first integrals are functionally independent. \square

We can now state the following.

Theorem 2. Consider the n -dimensional QP system (1) of matrix M . If $\text{rank}(M) = r < n$, then there exists a quasimonomial transformation that leads from such a system to an n -dimensional QP system of matrix

$$M_r = \begin{pmatrix} R_{r \times (m+1)} \\ O_{(n-r) \times (m+1)} \end{pmatrix}. \tag{12}$$

Since the proof relies on simple matrix algebra, we shall omit it.

It should be emphasized that, if $\text{rank}(B)$ is maximal for the original system, this will also be the case for the target QP system of r variables and m quasimonomials. Consequently, the reduction to maximal rank of M has been completed.

It is still possible that $\text{rank}(M)$ is maximal, but $\text{rank}(A)$ is not—for $m \geq n$, $\text{rank}(M) = n$ and $\text{rank}(A) = (n - 1)$. A new-time transformation of the form (5) will solve it if, in particular, we choose $\beta_i = -B_{ji}$, $i = 1, \dots, n$, for an appropriate value of j , $1 \leq j \leq m$. The result is a QP system for which both matrices M and A have maximal rank n . Notice that this new-time transformation does not change the rank of matrix B .

Consequently, we have demonstrated that every QP system can be reduced to an equivalent QP system with $m \geq n$ and matrices B , A and M of maximal rank n . Hereafter, it is assumed that the system under consideration complies to this standard form.

3. Reduction of the degree of nonlinearity

3.1. Algebraic theory

In this section we shall show how the degree of nonlinearity can be reduced by means of appropriate manipulations of a given QP system, the ultimate goal being a quadratic vector field.

The simplest case arises when $m = n$: B is an $n \times n$ invertible matrix, and we can set $C = B^{-1}$. The result is another flow for which $B' = I_n$, namely a Lotka–Volterra system. The reduction is thus achieved.

In the complementary case $m > n$, B is not square and cannot be reduced to diagonal form. The maximal reduction of the degree of nonlinearity proceeds as follows. We split B in two submatrices:

$$B = \begin{pmatrix} B_{n \times n} \\ B_{(m-n) \times n} \end{pmatrix}. \tag{13}$$

Since $\text{rank}(B) = n$ we can assume, without loss of generality, that $\text{rank}(B_{n \times n}) = n$. Then, if $C = B_{n \times n}^{-1}$, the result is a QP system for which:

$$B' = B \cdot C = \begin{pmatrix} I_n \\ B_{(m-n) \times n} \cdot B_{n \times n}^{-1} \end{pmatrix}. \tag{14}$$

In other words, only n quasimonomials in the vector field can be reduced to quadratic form in this case. The form of the $(m - n)$ remaining quasimonomials is fixed by $B_{(m-n) \times n} \cdot B_{n \times n}^{-1}$ and a reduction of the degree cannot be applied to them.

When $m > n$ a complete reduction of the original system to a Lotka–Volterra form is accomplished by performing an embedding. The process leading to (6) particularized to $p = m - n$. Here, $B_{m \times (m-n)}$ in (6) must be composed of arbitrary entries such that \tilde{B} is invertible. Then we have defined an expanded m -dimensional QP system and an invertible matrix \tilde{B} to which the procedure of the $m = n$ case can be applied. Consequently, a unique Lotka–Volterra representative can also be associated to system (1) in the case $m > n$: that of matrix $M_{LV} = \tilde{B} \cdot \tilde{M} = B \cdot M$.

We can now state the following new result for these systems.

Theorem 3. The target Lotka–Volterra system has $(m - n)$ independent first integrals, given by

$$F_i(\xi_1, \dots, \xi_m) = \xi_i^{-1} \prod_{j=1}^n \xi_j^{\alpha_{ij}} - 1 = 0 \quad n + 1 \leq i \leq m \quad (15)$$

where the constants α_{ij} , $n + 1 \leq i \leq m$, $1 \leq j \leq n$, satisfy the relations:

$$B_{il} = \sum_{j=1}^n \alpha_{ij} B_{jl} \quad 1 \leq l \leq n. \quad (16)$$

The proof is not especially involved, and we omit it.

Embedding (6) can actually be applied in such a way that the number k of new variables is smaller than $(m - n)$. Therefore, it will be possible to reduce to quadratic nonlinearity at most $(n + k)$ quasimonomials by means of a quasimonomial transformation. On the other hand, the resulting $(n + k)$ -dimensional QP system will have k independent first integrals of quasimonomial form introduced by the embedding. $\text{Rank}(M) = n$ for the target system and the explicit characterization of these k first integrals is given by theorem 1.

To summarize, the alternative steps are:

- (a) if the dimension is to be preserved: one quasimonomial transformation;
- (b) in those cases ($m > n$) where the dimension may be increased: add extra variables of constant value 1 and make an appropriate quasimonomial transformation.

3.2. Example 1

We shall illustrate the previous procedures with a system of relevance in the field of molecular physics, the Morse oscillator [21]. The system is given by:

$$\begin{aligned} \dot{x} &= y \\ \dot{y} &= -2d\alpha e^{-\alpha x} (1 - e^{-\alpha x}). \end{aligned} \quad (17)$$

We now perform a phase-space translation of magnitude c , followed by the introduction of a new variable $z = e^{-\alpha x}$. Thus:

$$\begin{aligned} \dot{x} &= x[x^{-1}y - cx^{-1}] \\ \dot{y} &= y[ay^{-1}z - aby^{-1}z^2] \\ \dot{z} &= z[\alpha c - \alpha y] \end{aligned} \quad (18)$$

where $a = -2db\alpha$ and $b = e^{\alpha c}$.

The maximal possible reduction in degrees without embedding corresponds to the choice:

$$C = \begin{pmatrix} -1 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & -1 & 1 \end{pmatrix}^{-1}. \tag{19}$$

After the transformation, the result is another QP system with exponents:

$$B' = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & -1 & 2 \\ 1 & -1 & 0 \end{pmatrix}. \tag{20}$$

We see that the last two quasimonomials have not been simplified by the transformation, as was to be expected.

We consider now the reduction via the Lotka–Volterra embedding. First, notice that from matrix B of (18), if we call ξ_i the quasimonomials, with $i = 1, \dots, 5$, we have

$$\xi_4 = \xi_1 \xi_2^{-1} \xi_3^2 \quad \xi_5 = \xi_1 \xi_2^{-1}. \tag{21}$$

Since the quasimonomials of the original QP system are the variables of the Lotka–Volterra system, these constraints will be present as first integrals in the final set of equations. We expand the characteristic matrices of (18) according to (6). After this embedding, the Lotka–Volterra system is given by matrix:

$$M_{LV} = \begin{pmatrix} 0 & -1 & c & a & -ab & 0 \\ 0 & -1 & c & 0 & 0 & 0 \\ \alpha c & 0 & 0 & -a & ab & -\alpha \\ 2\alpha c & 0 & 0 & -a & ab & -2\alpha \\ 0 & 0 & 0 & a & -ab & 0 \end{pmatrix}. \tag{22}$$

We observe that $\text{rank}(M_{LV}) = 3$. In particular, we have $(\text{row}4) = (\text{row}1) - (\text{row}2) + 2 \times (\text{row}3)$ and $(\text{row}5) = (\text{row}1) - (\text{row}2)$. After a straightforward integration of the corresponding evolution equations (see theorem 1 for further details) we recover the first integrals (21). This description of the system has the advantage of being purely quadratic.

We can also proceed from (18) to a partial embedding, for example the one for which the expanded matrices are:

$$\tilde{M} = \begin{pmatrix} 0 & 1 & -c & 0 & 0 & 0 \\ 0 & 0 & 0 & a & -ab & 0 \\ \alpha c & 0 & 0 & 0 & 0 & -\alpha \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad \tilde{B} = \begin{pmatrix} -1 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & -1 & 2 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix} \tag{23}$$

plus the initial condition $x_4(0) = 1$. We now take

$$C = \begin{pmatrix} -1 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & -1 & 2 & 1 \end{pmatrix}^{-1}. \tag{24}$$

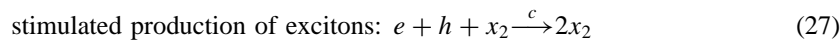
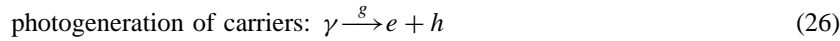
This leads to the following system:

$$\begin{aligned} \dot{z}_1 &= z_1[-z_1 + cz_2 + \alpha z_3 - abz_4] \\ \dot{z}_2 &= z_2[-z_1 + cz_2] \\ \dot{z}_3 &= z_3[\alpha c - \alpha z_3 + abz_4 - \alpha z_1 z_2^{-1}] \\ \dot{z}_4 &= z_4[2\alpha c - \alpha z_3 + abz_4 - 2\alpha z_1 z_2^{-1}] \end{aligned} \tag{25}$$

where four quasimonomials have been reduced. From matrix C we have $x_4 = x_4(0) = 1 = z_1^{-1}z_2z_3^{-2}z_4$, a first integral which is present in the target system, as inferred from the fact that (row4) = (row1) – (row2) + 2 × (row3). In this case we have a balance between the increase in the dimension and the expression of the flow in quadratic terms.

3.3. Example 2

As a second example, we shall consider a model describing sustained time-oscillations in the concentration of electron–hole pairs (x_1) and excitons (x_2) in an intrinsic semiconductor [22]. The process consists of the following steps:



When high-order kinetics is allowed in the model, the process is described by the equations:

$$\begin{aligned} \dot{x}_1 &= g - cx_1^2x_2 \\ \dot{x}_2 &= cx_1^2x_2 - \frac{kx_2}{(1 + qx_2)^m}. \end{aligned} \quad (29)$$

System (29) can be readily put into QP form by introducing a new variable such as $x_3 = (1 + qx_2)^{-1}$. The resulting flow is:

$$\begin{aligned} \dot{x}_1 &= x_1[gx_1^{-1} - cx_1x_2] \\ \dot{x}_2 &= x_2[cx_1^2 - kx_3^m] \\ \dot{x}_3 &= x_3[-cqx_1^2x_2x_3 + qkx_2x_3^{m+1}]. \end{aligned} \quad (30)$$

The three interactions originally presented in (29) correspond to the second, third and fourth quasimonomials of the QP system (30). More precisely, these quasimonomials can be seen as interactions *per capita*, as we have already pointed out [16]. Accordingly, we can particularize such interactions as the representative variables, by means of a quasimonomial transformation of the matrix:

$$C = \begin{pmatrix} 1 & 1 & 0 \\ 2 & 0 & 0 \\ 0 & 0 & m \end{pmatrix}^{-1}. \quad (31)$$

The transformed equations are:

$$\begin{aligned} \dot{y}_1 &= y_1[-cy_1 + cy_2 - ky_3 + gy_2^{-1/2}] \\ \dot{y}_2 &= y_2[-2cy_1 + 2gy_2^{-1/2}] \\ \dot{y}_3 &= y_3[-cqm y_1 y_2^{1/2} y_3^{1/m} + qkm y_1 y_2^{-1/2} y_3^{1+1/m}]. \end{aligned} \quad (32)$$

In this representation, the three *per capita* interactions (given by y_1 , y_2 and y_3) appear as linear quasimonomials. This means that we can alternatively describe the system in terms of rates of stimulated production and radiative decay of excitons, i.e. the fundamental physical processes, and this can be done while reducing the degree of nonlinearity of the model.

We can complete the reduction to quadratic (Lotka–Volterra) form. The resulting matrix is:

$$A_{LV} = \begin{pmatrix} -g & c & 0 & 0 & 0 & 0 \\ g & -c & c & -k & 0 & 0 \\ 2g & -2c & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -cqm & qkm \\ 2g & -2c & c & -k & -cq & qk \\ 0 & 0 & c & -k & -cq(1+m) & qk(1+m) \end{pmatrix}. \tag{33}$$

From matrix (33), the first integrals are $y_2 y_3^{1/2} y_4^{1/m} y_5^{-1}$, $y_2 y_3^{-1/2} y_4^{1+1/m} y_6^{-1}$ and $y_1 y_3^{1/2}$. This conclusion can also be anticipated from matrix B of (30), by following the same procedure as in example 1.

The last possibility is that of a partial embedding. We may, for instance, add one new variable:

$$\tilde{M} = \begin{pmatrix} 0 & g & -c & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & c & -k & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -cq & qk \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad \tilde{B} = \begin{pmatrix} -1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 \\ 2 & 0 & 0 & 0 \\ 0 & 0 & m & 0 \\ 2 & 1 & 1 & 0 \\ 0 & 1 & m+1 & 0 \end{pmatrix}. \tag{34}$$

Our quasimonomial transformation is now the one given by:

$$C = \begin{pmatrix} -1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 \\ 2 & 0 & 0 & 0 \\ 0 & 0 & m & 0 \end{pmatrix}^{-1}. \tag{35}$$

The final system is then:

$$\begin{aligned} \dot{z}_1 &= z_1[-gz_1 + cz_2] \\ \dot{z}_2 &= z_2[gz_1 - cz_2 + cz_3 - kz_4] \\ \dot{z}_3 &= z_3[2gz_1 - 2cz_2] \\ \dot{z}_4 &= z_4[-cqmz_2z_3^{1/2}z_4^{1/m} + qkmz_2z_3^{-1/2}z_4^{1+1/m}]. \end{aligned} \tag{36}$$

In this case, we describe the system by looking at the full set of interactions, including also the *per capita* rate of photogeneration of carriers (z_1). It can be easily checked that the first integral $z_1 z_3^{1/2}$ has been introduced in the process. However, now the degree of nonlinearity of the description is smaller than in (32).

4. Reduction of the number of nonlinear terms

4.1. Algebraic theory

The complementary approach to the problem of structural simplification of a nonlinear system proceeds to the reduction of the total number of nonlinear terms constituting each component of the vector field.

For $m = n$, it is possible to redistribute the quasimonomials assigning one of them to each equation. A is invertible and we can therefore set $C = A$: $A' = I_n$ for the target flow, yielding a system for which only one nonlinear term per equation is present. This system is called the *unimonomial system*. The reduction to this form has been useful in the study of

integrability properties of ODEs [2] as well as in the construction of models in theoretical biochemistry [13].

In the case $m > n$ it is no longer possible to reallocate m quasimonomials in n equations by means of a quasimonomial transformation. The maximal reduction that can be achieved in this way proceeds as follows. Let A be: $A = (A_{n \times n} | A_{n \times (m-n)})$. Since $\text{rank}(A)$ is maximal, we can assume that $A_{n \times n}$ is invertible. Then, if we set $C = A_{n \times n}$ (a choice that determines C completely) the result is a QP system with $A' = (I_n | A_{n \times n}^{-1} \cdot A_{n \times (m-n)})$.

In other words, only n quasimonomials can be doled out among the n equations in this case. The redistribution of the remaining $(m - n)$ quasimonomials cannot be controlled and depends on the entries of the initial matrix A .

It is necessary to increase to m the number of equations, before a complete redistribution of the m quasimonomials, by means of transformation (7), particularized to $p = (m - n)$. The entries of $M_{(m-n) \times (m+1)}$ in (7) are in principle arbitrary, but should nevertheless be chosen appropriately to ensure maximal rank for the expanded matrix \tilde{A} . The problem is thus reduced to the previous situation $m = n$.

The consequence of this simplification of the system is twofold. First, the dimension has been increased. Secondly, the information from the original system is intermingled with spurious components originated from the embedding process, in such a way that both expanded and original systems are not topologically equivalent. It is clear from equation (7) that the information is not necessarily confined to a submanifold of the m -dimensional phase space, as was the case in the Lotka–Volterra embedding. Consequently, the original topology of the starting n -dimensional phase space will not be preserved, in general, in an n -dimensional submanifold of the target m -dimensional phase space; the matter being further worsened after any quasimonomial transformation acting upon the expanded system.

We shall analyse this problem in detail here for the first time. We shall demonstrate that, although the topological equivalence is not preserved in the process, the information corresponding to the original system can always be retrieved in each step of the procedure by means of a simple projection technique.

Let us make some definitions; we will call \mathbf{x} the m -dimensional vector

$$\mathbf{x} = \left(x_1(t), \dots, x_n(t), \overbrace{1, \dots, 1}^{m-n} \right)^T \quad (37)$$

which is essentially the solution to the original n -dimensional problem (1), and

$$\mathbf{x}_{\text{exp}} = (x_1(t), \dots, x_m(t))^T \quad (38)$$

the corresponding solution of the expanded system (7) (particularized to $p = m - n$). Since all variables are assumed to be strictly positive, we can equivalently deal with the logarithms $\ln \mathbf{x}$ and $\ln \mathbf{x}_{\text{exp}}$ of the vectors. Then we can retrieve the solution \mathbf{x} from \mathbf{x}_{exp} by means of the matrix identity

$$\ln \mathbf{x} = P_n \cdot \ln \mathbf{x}_{\text{exp}} \quad (39)$$

where $P_n = \text{diag}(I_n, O_{(m-n) \times (m-n)})$. P_n just projects, in logarithmic space, the m -dimensional solution onto the hyperplane $\ln x_{n+1} = \dots = \ln x_m = 0$.

We can now consider the effect of a quasimonomial transformation performed over system (7) with $p = m - n$. We will denote as \mathbf{z} , \mathbf{z}_{exp} , the transformed trajectories from \mathbf{x} , \mathbf{x}_{exp} , respectively. The following relations hold:

$$\ln \mathbf{x} = C \cdot \ln \mathbf{z} \quad \ln \mathbf{x}_{\text{exp}} = C \cdot \ln \mathbf{z}_{\text{exp}} \quad (40)$$

From this, together with (39), the following identity can be deduced:

$$\ln \mathbf{z} = C^{-1} \cdot P_n \cdot C \cdot \ln \mathbf{z}_{\text{exp}} \equiv P'_n \cdot \ln \mathbf{z}_{\text{exp}} \quad (41)$$

Equation (41) shows how P_n is transformed under a quasimonomial transformation of matrix C . It is then clear from definition (3) that z belongs to the submanifold of \mathcal{R}^m

$$\prod_{j=1}^m z_j^{C_{ij}} = 1 \quad i = n + 1, \dots, m \quad (42)$$

or

$$\sum_{j=1}^m C_{ij} \ln z_j = 0 \quad i = n + 1, \dots, m. \quad (43)$$

In fact, this submanifold is the one obtained by transforming the surface containing the original n -dimensional phase space, namely $x_{n+1} = \dots = x_m = 1$, by means of the quasimonomial transformation. It is not difficult to see that P'_n , as given by equation (41), is nothing else than the projection matrix on hyperplane (43) of \mathcal{R}^m . Substituting (41) into (43) we have

$$\sum_{j=1}^m C_{ij} \ln(z_n)_j = \sum_{j=1}^m (P_n \cdot C)_{ij} \ln(z_m)_j = 0 \quad \text{if } i > n \quad (44)$$

since $(P_n \cdot C)_{ij} = 0$ if $i > n$. Consequently, this demonstrates that the original phase space is topologically equivalent to the *projection* of the transformed trajectories $\ln z_m(t)$ onto the n -dimensional manifold (43). However, it must be pointed out that this does *not* imply that the single quasimonomial form embedding preserves topological equivalence between the original n -dimensional phase space and some particular submanifold of \mathcal{R}^m . Nevertheless, this constructive procedure permits to discern relevant from spurious information at every stage of the manipulation of the equations. In particular, no inversion of the embedding procedure is required for the retrieval of the significant information of the system. The explicit knowledge of the projection matrix P'_n allows direct access to it, once the solution $z_m(t)$ has been integrated.

We close this section by adding that the unimonomial embedding can be performed only partially. Let k be the number of extra equations in (7), $1 \leq k < (m - n)$. In this case, only $(n + k)$ quasimonomials will be amenable of redistribution among the equations. It is also clear that appropriate projection operators must be introduced in order to screen the relevant information.

Again, we summarize the main alternative steps.

- (a) If the dimension is to be preserved: a quasimonomial transformation.
- (b) If the dimension can be increased, the sequence is:
 - (b.1) add new variables decoupled from the original ones;
 - (b.2) make an appropriate quasimonomial transformation;
 - (b.3) 'keep track' of the relevant information: find the projection matrix.

4.2. Example 3

Let us consider the Brusselator equations [23], a model system for the Belousov–Zhabotinskii reaction. In QP form, the equations are:

$$\begin{aligned} \dot{x}_1 &= x_1[-(b + 1) + x_1 x_2 + a x_1^{-1}] \\ \dot{x}_2 &= x_2[b x_1 x_2^{-1} + x_1^2]. \end{aligned} \quad (45)$$

If we proceed without embedding, two quasimonomials can be redistributed at will among the equations. We may select the quasimonomial transformation of matrix:

$$C = \begin{pmatrix} 1 & 0 \\ 0 & b \end{pmatrix}. \quad (46)$$

For the reduced QP system we have:

$$M' = \begin{pmatrix} -(b+1) & 1 & 0 & a & 0 \\ 0 & 0 & 1 & 0 & -1/b \end{pmatrix}. \quad (47)$$

In contrast, if we want a complete redistribution of the quasimonomials, an embedding must be applied, for instance the following one:

$$\tilde{M} = \begin{pmatrix} -(b+1) & 1 & 0 & a & 0 \\ 0 & 0 & b & 0 & -1 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad \tilde{B} = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 2 & 0 & 0 & 0 \end{pmatrix}. \quad (48)$$

The final unimonomial system, which is reached after a quasimonomial transformation of matrix $C = \tilde{A}$, is:

$$\begin{aligned} \dot{z}_1 &= z_1[-(b+1) + z_1 z_2^b z_3^a z_4^{-1}] \\ \dot{z}_2 &= z_2[z_1 z_2^{-b} z_3^a z_4] \\ \dot{z}_3 &= z_3[z_1^{-1} z_3^{-a}] \\ \dot{z}_4 &= z_4[z_1^2 z_3^{2a}]. \end{aligned} \quad (49)$$

This is an optimal flow, in the sense that only one nonlinear term is present per equation. We retrieve the original trajectories of system (45) if we project the logarithms of the solutions of (48) onto the plane $\{\ln(x_3) = 0, \ln(x_4) = 0\}$, i.e. by means of the projection matrix:

$$P_2 = \begin{pmatrix} I_2 & \\ & O_{2 \times 2} \end{pmatrix}. \quad (50)$$

Under the quasimonomial transformation leading to the reduced system (49) this operator is transformed to:

$$P_2' = C^{-1} \cdot P_2 \cdot C = \begin{pmatrix} 1 & 0 & a & 0 \\ 0 & 1 & 0 & -1/b \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (51)$$

This operator still projects onto the plane $\{\ln(z_3) = 0, \ln(z_4) = 0\}$. Consequently, although the flow is four dimensional, only the knowledge of the first two variables is necessary for the investigation of the topology of the initial flow (45), since such topology is equivalent to that obtained when $z_1(t)$ and $z_2(t)$ are represented on \mathcal{R}^2 . Another way of expressing this is by noticing that the projection plane $\{\ln(x_3) = 0, \ln(x_4) = 0\}$ remains invariant under the quasimonomial transformation we perform.

The third alternative is that of a partial embedding. One possibility for adding the new variable is:

$$\tilde{M} = \begin{pmatrix} -(b+1) & 1 & 0 & a & 0 \\ 0 & 0 & b & 0 & -1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix} \quad \tilde{B} = \begin{pmatrix} 1 & 1 & 0 \\ 1 & -1 & 0 \\ -1 & 0 & 0 \\ 2 & 0 & 0 \end{pmatrix}. \quad (52)$$

The partially reduced system is then:

$$\begin{aligned} \dot{y}_1 &= y_1[-(b+1) + y_1 y_2^b y_3^a] \\ \dot{y}_2 &= y_2[y_1 y_2^{-b} y_3^a - (1/b)y_1^2 y_3^{2a}] \\ \dot{y}_3 &= y_3[y_1^{-1} y_3^{-a}]. \end{aligned} \quad (53)$$

This system represents a compromise between (47) and (49). The projection plane $\{\ln(x_3) = 0\}$ is again invariant under the quasimonomial transformation:

$$P_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \implies P'_2 = C^{-1} \cdot P_2 \cdot C = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & 0 & 0 \end{pmatrix}. \tag{54}$$

Again the third variable is to be discarded.

It should be emphasized that, along this example, a great simplification of the procedure given in section 4.1 comes from the fact that the projection plane remains invariant under the quasimonomial transformation and, consequently, the projection procedure reduces, in the final system, to the suppression of the spurious variables. Such a feature is *not* particular to this example. The unimonomial embedding can always be chosen in such a way that this property holds.

4.3. Example 4

We shall now apply our technique to a system which models the nonlinear interaction of three waves (see [18] and references therein):

$$\begin{aligned} \dot{x}_1 &= x_1 \left[\lambda_1 + \sum_{j=1}^3 N_{1j} x_j^2 + \gamma x_1^{-1} x_2 x_3 \right] \\ \dot{x}_2 &= x_2 \left[\lambda_2 + \sum_{j=1}^3 N_{2j} x_j^2 \right] \\ \dot{x}_3 &= x_3 \left[\lambda_3 + \sum_{j=1}^3 N_{3j} x_j^2 \right]. \end{aligned} \tag{55}$$

Here the dependent variables x_i describe the amplitudes of the three interacting modes; the λ 's, when negative, account for dissipation; the N_{ij} denote modes of competition among waves; finally, the model includes a resonance term, which is that dependent on γ .

Equations (55) have 10 nonlinear terms. A good possibility for simplifying them proceeds without embedding, by means of a quasimonomial transformation of matrix:

$$C = \begin{pmatrix} N_{11} & N_{12} & N_{13} \\ N_{21} & N_{22} & N_{23} \\ N_{31} & N_{32} & N_{33} \end{pmatrix}. \tag{56}$$

The new vector field is given by matrices of the form:

$$M' = \begin{pmatrix} \lambda'_1 & 1 & 0 & 0 & \gamma'_1 \\ \lambda'_2 & 0 & 1 & 0 & \gamma'_2 \\ \lambda'_3 & 0 & 0 & 1 & \gamma'_3 \end{pmatrix} \quad B' = \begin{pmatrix} 2N_{11} & 2N_{12} & 2N_{13} \\ 2N_{21} & 2N_{22} & 2N_{23} \\ 2N_{31} & 2N_{32} & 2N_{33} \\ \nu_1 & \nu_2 & \nu_3 \end{pmatrix} \tag{57}$$

where $\nu_j = -N_{1j} + N_{2j} + N_{3j}$, and the new system will be:

$$\begin{aligned} \dot{y}_1 &= y_1 [\lambda'_1 + y_1^{2N_{11}} y_2^{2N_{12}} y_3^{2N_{13}} + \gamma'_1 y_1^{\nu_1} y_2^{\nu_2} y_3^{\nu_3}] \\ \dot{y}_2 &= y_2 [\lambda'_2 + y_1^{2N_{21}} y_2^{2N_{22}} y_3^{2N_{23}} + \gamma'_2 y_1^{\nu_1} y_2^{\nu_2} y_3^{\nu_3}] \\ \dot{y}_3 &= y_3 [\lambda'_3 + y_1^{2N_{31}} y_2^{2N_{32}} y_3^{2N_{33}} + \gamma'_3 y_1^{\nu_1} y_2^{\nu_2} y_3^{\nu_3}]. \end{aligned} \tag{58}$$

The new variables are $y_i = x_1^{d_{i1}} x_2^{d_{i2}} x_3^{d_{i3}}$, where the d_{ij} are the entries of $D = C^{-1}$. Therefore, they are nonlinear combinations of the original amplitudes x_i , the exponents being functions of the competition coefficients N_{ij} . Then, our redefinition of the amplitudes is such that for

the new, equivalent set of amplitudes y_i , the competition with the other waves is summarized in only *one* nonlinear term per wave. This new representation is not optimal from the point of view of the resonance, which is now present in all equations. The overall result, however, is that of a simplification, since the number of nonlinear terms in the new flow is only six.

The remaining possibility is that of a complete embedding:

$$\tilde{M} = \begin{pmatrix} \lambda_1 & N_{11} & N_{12} & N_{13} & \gamma \\ \lambda_2 & N_{21} & N_{22} & N_{23} & 0 \\ \lambda_3 & N_{31} & N_{32} & N_{33} & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad \tilde{B} = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ -1 & 1 & 1 & 0 \end{pmatrix}. \quad (59)$$

The quasimonomial transformation now is evidently that of matrix $C = \tilde{A}$. The resulting matrices are of the form:

$$\tilde{M}' = \begin{pmatrix} \tilde{\lambda}_1 & 1 & 0 & 0 & 0 \\ \tilde{\lambda}_2 & 0 & 1 & 0 & 0 \\ \tilde{\lambda}_3 & 0 & 0 & 1 & 0 \\ \tilde{\lambda}_4 & 0 & 0 & 0 & 1 \end{pmatrix} \quad \tilde{B}' = \begin{pmatrix} 2N_{11} & 2N_{12} & 2N_{13} & 2\gamma \\ 2N_{21} & 2N_{22} & 2N_{23} & 0 \\ 2N_{31} & 2N_{32} & 2N_{33} & 0 \\ v_1 & v_2 & v_3 & -\gamma \end{pmatrix}. \quad (60)$$

The system has thus achieved the maximal simplification:

$$\begin{aligned} \dot{z}_1 &= z_1[\tilde{\lambda}_1 + z_1^{2N_{11}} z_2^{2N_{12}} z_3^{2N_{13}} z_4^{2\gamma}] \\ \dot{z}_2 &= z_2[\tilde{\lambda}_2 + z_1^{2N_{21}} z_2^{2N_{22}} z_3^{2N_{23}}] \\ \dot{z}_3 &= z_3[\tilde{\lambda}_3 + z_1^{2N_{31}} z_2^{2N_{32}} z_3^{2N_{33}}] \\ \dot{z}_4 &= z_4[\tilde{\lambda}_4 + z_1^{v_1} z_2^{v_2} z_3^{v_3} z_4^{-\gamma}]. \end{aligned} \quad (61)$$

From the physical point of view, both types of interactions among waves (competition among modes and resonance) are now described simultaneously by one single nonlinear term in each of the equations. This can be clearly inferred from the form of the exponents of the quasimonomials in (61). In this case, the simplification of the number of nonlinear terms is the maximal possible, since only four of them are present in system (61).

From the form of matrix C , we need not compute explicitly the projection matrix to find the projection plane: it must be $\{\ln(z_4) = 0\}$, since the plane $\{\ln(x_4) = 0\}$ is invariant under the quasimonomial transformation.

5. Final remarks

We may conclude by a few remarks on the unified scheme presented here when compared with other approaches to the case problems. In the introduction we mentioned the work of Kerner [11] on the reduction of general systems of ODEs to what he calls ‘elemental Riccati systems’ (ERS), the vector field which is strictly quadratic—with simple arrays of coefficients that are either zero or unity. Let us consider Kerner’s example, which starts from the one-dimensional standard cubic equation:

$$\dot{x} = a_0 + a_1x + a_2x^2 + a_3x^3 \quad (62)$$

and produces an 11-dimensional ERS

$$\dot{z}_\alpha = \sum_{\beta, \gamma=1}^{11} E_{\alpha\beta\gamma}^* z_\beta z_\gamma \quad \alpha = 1, \dots, 11. \quad (63)$$

The QP formalism, when applied to (62), leads to a three-dimensional Lotka–Volterra system, a much smaller dimensionality, indeed. Both the ERS and Lotka–Volterra systems

are compact formats, liable to be analysed in a purely algebraic context. Notwithstanding these similarities, there is a particularity which favours the QP formalism. Kerner's approach proceeds in two steps: a rule of thumb transformation to a Riccati system, followed by a sequence of algebraic operations to produce the final ERS form. In contrast, in the QP formalism the procedure is systematically carried out from the very beginning through simple matrix operations.

Finally, a similar assessment can be made when it comes to comparing known alternative approaches for a simplification of the number of nonlinear terms in each component of the flow. We may recall the *ad hoc* method of Savageau and collaborators [1, 12], a heuristic technique which raises serious doubts about its mathematical consistency. It strongly relies on arbitrary user-dependent choices of additional variables that lead to manifold systems complying to a specified format. This is in opposition to the unique unimonomial form we are able to construct by the technique of section 4.1.

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