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Two approaches for testing identifiability and corresponding algorithms

Lilianne Denis-Vidal*, Ghislaine Joly-Blanchard†, Céline Noiret †, Michel Petitot*

†University of Technology of Compiègne, France

* University of Sciences and Tech. Lille, France

lilianne.denis-vidal@math.univ-lille1.fr, ghislaine.joly-blanchard@utc.fr, celine.noiret@utc.fr, michel.petitot@lifl.fr

Abstract

This paper considers two different methods in the analysis of nonlinear controlled dynamical system identifiability. The corresponding identifiability definitions are not equivalent. Moreover one is based on the construction of an input-output ideal and the other on the similarity transformation theorem. Our aim is to develop algorithms which give identifiability results from both approaches. Differential algebra theory allows realization of such a project. In order to state these algorithms, new results of differential algebra must be proved. Then the implementation of these algorithms is done in a symbolic computation language.

Key words - *Nonlinear dynamical systems, Structural identifiability, Symbolic manipulation.*

Introduction

In this paper, two types of models are introduced in order to analyze nonlinear controlled dynamical system identifiability.

Firstly, the initial conditions are ignored:

$$\Sigma^\theta \begin{cases} \dot{x}(t, \theta) = f(x(t, \theta), \theta) + u(t)g(x(t, \theta), \theta), \\ y(t, \theta) = h(x(t, \theta), \theta). \end{cases} \quad (1)$$

Secondly, the initial conditions are known:

$$\Sigma_{x_0(\theta)}^\theta \begin{cases} \dot{x}(t, \theta) = f(x(t, \theta), \theta) + u(t)g(x(t, \theta), \theta), \quad x(0, \theta) = x_0(\theta), \\ y(t, \theta) = h(x(t, \theta), \theta). \end{cases} \quad (2)$$

In both cases, $x(t, \theta) \in \mathbb{R}^n$, $y(t, \theta) \in \mathbb{R}^m$, $u(t) \in \mathbb{R}$ denote the state variables, the measured outputs and the input respectively. The parameter vector θ is in Ω_q , an open subset of \mathbb{R}^q . The single-input case is taken into account for notational simplicity; all the results can be generalized readily.

The functions $f(x, \theta)$, $g(x, \theta)$ and $h(x, \theta)$ are real and rational and may depend on a real constant vector denoted by a . In this case the set K corresponds to $\mathbb{R}(a)$ (i.e. the field generated by \mathbb{R} and a), otherwise K corresponds to \mathbb{R} .

In the 90's Diop and Fliess [6], Fliess and Glad [8], Ljung and Glad [13] and Ollivier [15] proposed a new approach of identifiability, based on differential algebra. The initial conditions are ignored as they are in the model Σ^θ . Thus, the solutions of model equations may be non-unique and some solutions might be of a degenerate character. Therefore, the concept of non-degenerate solutions $\bar{x}(\theta, u)$ and $\bar{y}(\theta, u)$ has to be considered and the definition introduced in [13] is adopted here:

Definition 0.1 *The model Σ^θ is globally identifiable at $\theta \in \Omega_q$ if for any $\tilde{\theta} \in \Omega_q$, $\tilde{\theta} \neq \theta$, there exists a control u such that $\bar{y}(\theta, u) \neq \bar{y}(\tilde{\theta}, u)$ and $\bar{y}(\theta, u) \cap \bar{y}(\tilde{\theta}, u) = \emptyset$. It is locally identifiable at $\theta \in \Omega_q$ if there exists an open neighborhood W of θ such that Σ^θ is globally identifiable at θ with Ω_q restricted to W .*

Now, let us introduce some useful notations.

- A *differential ring (respectively field)* is a ring (respectively field) endowed with a set of derivations which commute pairwise.
- Let V be a set of differential indeterminates and Δ be a set of derivations which commute pairwise. We denote by Θ the commutative monoid generated by Δ and by ΘV the set of all the derivatives $\phi v, \phi \in \Theta, v \in V$. Given a field K , $K\{V\}$ is the *differential ring* of the differential polynomials built over the alphabet ΘV with coefficients in K .
- The differential field generated by K and \tilde{V} is denoted by $K\langle\tilde{V}\rangle$, $\tilde{V} \subset V$ and, by definition, it is equal to $K(\Theta\tilde{V})$ (i.e. the smallest field which contains K and $\Theta\tilde{V}$).

Since the functions f, g and h are rational functions, the identifiability techniques based on differential algebra are well appropriate. Indeed, the controlled system is considered as a set of variables (indeterminates) $\{u, x, y, \theta\}$ linked by a differential ideal. Ljung and Glad [13] and Ollivier [15] exploited the concept of *characteristic set*. The characteristic set of the differential ideal, defined by dynamical system equations, is a finite set of polynomials which summarizes the whole information contained in the differential ideal. Ljung and Glad perform a characteristic set which leads to the expression of each parameter as a rational function of u, y and their derivatives. Thus, they have shown the following results:

- A system is locally identifiable if and only if any parameter θ_i is differentially algebraic over $K\langle u, y \rangle$. It is the definition of the *algebraic identifiability* of Diop and Fliess [6], which is strongly connected to the *nonlinear observability*.
- A system is globally identifiable if any parameter θ_i belongs to the field $K\langle u, y \rangle$. It is the definition of the *rational identifiability* of Diop and Fliess [6].

Ljung and Glad's approach often leads to cumbersome computation.

Ollivier derives the identifiability from the computation of the characteristic set corresponding to the input-output ideal of differential algebraic relations between u, y and θ . The identifiability is obtained after analyzing this characteristic set.

In the first proposed method of this paper, the notion of *characteristic presentation* is considered instead of characteristic set because it supplies an effective way for testing the equality of some ideals. The resulting algorithm is implemented in MAPLE, a symbolic computation language, and uses the package DIFFALG especially.

On the other hand, it is noticeable that Definition 0.1 is well in line with the usual analytic definition of global (local) identifiability valid only for the system $\Sigma_{x_0(\theta)}^\theta$ (i.e. the initial conditions are known after selecting $\theta \in \Omega_q$):

Definition 0.2 *The model $\Sigma_{x_0(\theta)}^\theta$ is globally identifiable at $\theta \in \Omega_q$ if for any $\tilde{\theta} \in \Omega_q, \tilde{\theta} \neq \theta$ there exists a control u , such that $\Sigma_{x_0(\theta)}^\theta$ and $\Sigma_{x_0(\tilde{\theta})}^{\tilde{\theta}}$ yield different outputs. It is locally identifiable at $\theta \in \Omega_q$ if there exists an open neighborhood W of θ such that $\Sigma_{x_0(\theta)}^\theta$ is globally identifiable at θ with Ω_q restricted to W .*

In most models there exist atypical points in Ω_q where the model is unidentifiable. Definitions 0.1 and 0.2 should be generically extended so that $\Sigma_{x_0(\theta)}^\theta$ (or Σ^θ) is said to be *globally structurally identifiable* if it is globally identifiable at all $\theta \in \Omega_q$ except at the points of a subset of zero measure in Ω_q .

Now, we introduce a second identifiability approach which is a nonlinear counterpart of the similarity transformation approach [19] and is based on the local state isomorphism theorem [7], [16]. It leads to the solution of a system of partial differential equations (PDE). This is an efficient method for controlled models.

In theory, one has to solve this partial differential system but an alternative is proposed here. Indeed the originality of our process is to solve the identifiability problem without solving (in the analytic sense) this partial differential system. To do that, a link between the integrability constraints of the partial differential system and the identifiability properties of the original system is established. It leads to an algorithm which is implemented in MAPLE VII.

The paper is organized as follows. First, Section 1 mentions some results necessary for the development of the first identifiability algorithm. Then Section 2 shows a necessary and sufficient identifiability condition which justifies the second algorithm. Lastly, two examples compare the performances of both algorithms.

1 Input-output ideal approach

1.1 Description

The system Σ^θ can be rewritten as a differential polynomial system that will be completed with $\dot{\theta}_i = 0, i = 1, \dots, q$. The resulting system Γ can be described by the following polynomial equations and inequations:

$$\Gamma \begin{cases} p(\dot{x}, x, u, \theta) = 0, \\ q(x, y, \theta) = 0, \\ r(x, y, \theta) \neq 0, \\ \dot{\theta}_i = 0, i = 1, \dots, q. \end{cases} \quad (3)$$

Thus, the functions $x_j, j = 1 \dots n$ are to be differentially algebraic over $K \langle u, \theta \rangle$, and so are the functions $y_i, i = 1 \dots m$. The input u is assumed to be differentially transcendent. In this context, a solution of Γ is a quadruplet of functions (x, y, u, θ) satisfying all the model equations.

\mathcal{I} is the radical of the differential ideal generated by the polynomials of Γ . From the ranking

$$[\theta] \prec [y, u] \prec [x] \quad (4)$$

that eliminates state variables and from the equations of Γ , characteristic presentations corresponding to \mathcal{I} are computed.

The proofs of the two following propositions, given in [14] are very technical and not constructive relatively to algorithm elaboration.

Proposition 1.1 *If \mathcal{I} , endowed with the ranking (4), admits a characteristic presentation, this presentation has the following form:*

$$\dot{\theta}_1, \dots, \dot{\theta}_q, P_1(y, u, \theta), \dots, P_m(y, u, \theta), Q_1(y, u, \theta, x), \dots, Q_n(y, u, \theta, x), \quad (5)$$

where the leader of the polynomial P_k is y_k for $k = 1, \dots, m$, and where the leader of the polynomial Q_j is x_j for $j = 1, \dots, n$.

In general, \mathcal{I} should be written as the intersection of regular differential ideals, each one admitting a characteristic presentation. However in the following, \mathcal{I} , endowed with the ranking (4), is assumed to be a regular ideal presented by a characteristic presentation \mathcal{C} . This assumption is not so restrictive. Indeed in the opposite case, the next proposition must be applied to each system corresponding to each component of the decomposition of the ideal.

Now let us introduce a few notations:

- L is the set of the leaders of the elements of \mathcal{C} , N denotes the other derivatives occurring in \mathcal{C} and $K[N]$ is the polynomial ring built over N with coefficients in K .
- $\mathcal{C}(\theta)$ is the characteristic presentation \mathcal{C} evaluated in the particular value of parameter θ .
- \mathcal{I}_θ is the radical of the differential ideal generated by Γ for the particular value of parameter θ and \mathcal{C}_θ is the characteristic presentation associated with the ranking $[y, u] \prec [x]$.

To avoid the evaluation of $\mathcal{C}(\theta)$ at each value of parameters, the following result gives a sufficient condition for the equality $\mathcal{C}_\theta = \mathcal{C}(\theta)$.

Proposition 1.2 *Let $\mathcal{C} = \{c_1, \dots, c_{m+n}, \dot{\theta}_1, \dots, \dot{\theta}_q\}$ be the characteristic presentation of the differential ideal \mathcal{I} endowed with the ranking (4).*

If, for every $\theta \in \Omega_q$ and for every $i = 1, \dots, m+n$, the initial of $c_i(\theta) \in \mathcal{C}(\theta)$ is not equal to zero and none of its factors ($\neq 1$) is a divisor of all the other coefficients of $c_i(\theta) \in K[N]$, then $\mathcal{C}_\theta = \mathcal{C}(\theta)$ for all $\theta \in \Omega_q$.

Now let us introduce \mathcal{I}_θ^{io} , the ideal obtained after eliminating state variables. Thus the set $C_\theta^{io} = C_\theta \cap K(\theta)\{u, y\}$ is a characteristic presentation of the ideal \mathcal{I}_θ^{io} , called *the input-output characteristic presentation*. As a consequence of Proposition 1.1, \mathcal{I}_θ^{io} contains the polynomials $P_i, i = 1 \dots m$.

The next proposition is valid under the assumption that there exists some generic solution of Σ^θ . A solution is called *generic* if it does not verify any equation out of the ideal's equations [15] (as a consequence it is also a non-degenerate solution). The genericity assumption is difficult to test but strong accessibility from every initial condition in a dense open subset of \mathbb{R}^n implies this property. Moreover, strong accessibility is obtained by the strong accessibility rank criterion (SARC) [18] at every initial condition of this dense open subset.

Proposition 1.3 *Let us assume that there exists some generic solution of Σ^θ . Then Σ^θ is globally identifiable at θ , in the sense of Definition 0.1, if and only if for every $\bar{\theta} \in \Omega_q$ ($\bar{\theta} \neq \theta$), the two corresponding input-output characteristic presentations (C_θ^{io} and $C_{\bar{\theta}}^{io}$) are distinct.*

Remark 1.1 *The previous proposition can be formulated in the equivalent form: if there exists a generic solution of Σ^θ , then Σ^θ is globally identifiable at θ , if and only if*

$$\forall \bar{\theta} \in \Omega_q \quad C_\theta^{io} = C_{\bar{\theta}}^{io} \Rightarrow \theta = \bar{\theta}.$$

The proof of the previous proposition is like the proof of Theorem 6 in Ollivier [15]. The only difference concerns the characteristic set or presentation.

1.2 Algorithm

The polynomials $P_i, i = 1 \dots m$, of C_θ^{io} can be seen as polynomials in y and their derivatives with coefficients in $K(\theta)$. In the following, those polynomials will be written as

$$P_i(y, u) = m_0(y, u) + \sum_{k=1}^{n_i} p_k^i(\theta) m_k^i(y, u).$$

Now let us present the algorithm that we have implemented in MAPLE VII. It will be referred to it as **Algo1**. Let us remark Steps 4 and 7 of Algo1 are based on Rosenfeld-Groebner algorithm which has been realized by F. Boulier in MAPLE VII [2].

Data: f, g and h .

Step 1 The software rewrites the original system Σ^θ as the differential polynomial system Γ defined by (3).

Step 2 The existence of a generic solution is validated by checking the SARC.

Step 3 The field of constants K is given and a standard ranking is implicitly introduced. It is possible to select a most suitable ranking by a careful analysis of the system.

Step 4 Rosenfeld-Groebner algorithm computes all the input-output characteristic presentations (it is possible to compute only the general input-output characteristic presentation). Then an input-output characteristic presentation is chosen by the user.

Step 5 The values of θ for which the polynomials P_i are not primitive over $K[N]$ (i.e the assumptions of proposition 1.2 are not satisfied) are computed.

Step 6 This step saves the coefficients $p_k^i(\theta)$ in a list called the "exhaustive summary". It is simplified in order to extract its smallest generator system in terms of degree, number of monomials,...

Step 7 The exhaustive summary is analyzed by Rosenfeld-Groebner algorithm; the following system:

$$\begin{cases} p_k^i(\theta) = p_k^i(\bar{\theta}), k = 1, \dots, n_i, i = 1 \dots, m \\ \bar{\theta}_i = 0, i = 1, \dots, q \end{cases} \quad (6)$$

is solved in the differential field $K(\theta) \langle \bar{\theta} \rangle$ with the standard ranking (or a most suitable ranking given by the user):

$$[\bar{\theta}_1] \prec [\bar{\theta}_2] \prec [\dots] \prec [\bar{\theta}_q] \quad (7)$$

In order to simplify the computation, the pure transcendental field extension $K(\theta)$ is considered as a field of coefficients; it leads to a structural identifiability.

At the end of this step results of identifiability are provided.

Finally, note that if Algo1 does not successfully terminate because the computation of the input-output characteristic presentation is too complex or the analysis of the exhaustive summary fails, it can be reapplied by using a different ranking in steps 4 or (and) 7.

Algo1 has been implemented in MAPLE VII and runs on any Pentium PC.

2 Similarity transformation approach

In this section, the following assumptions are assumed: The functions $f(\cdot, \theta)$ and $h(\cdot, \theta)$ are real, rational and analytic for every $\theta \in \mathcal{U}_p$ on M (a connected open subset of \mathbb{R}^n such that $x(t, \theta) \in M$ for every $\theta \in \mathcal{U}_p$ and every $t \in [0, T]$); $f(x_0(\theta), \theta) \neq 0$ for every $\theta \in \mathcal{U}_p$; the input vector u is in $\mathcal{U}[0, T]$, the set of bounded and measurable functions defined on the time interval $[0, T]$; the initial state $x_0(\theta)$ is well defined after selecting θ .

Finally, the system $\Sigma_{x_0(\theta)}^\theta$ is assumed to be locally reduced at $x_0(\theta)$ for all $\theta \in \Omega_q$.

2.1 Description

The parameter identifiability can be obtained by using the local state isomorphism theorem which leads to the following result [17]:

Theorem 2.1 *The model $\Sigma_{x_0(\theta)}^\theta$ is assumed to be locally reduced at $x_0(\theta)$ for all $\theta \in \Omega_q$. Consider the parameter values θ and $\bar{\theta}$ in Ω_q , an open neighborhood V of $x_0(\theta)$ in M and any analytical mapping $\lambda: V \rightarrow \mathbb{R}^n$ defined in $V \subset \mathbb{R}^n$ such that*

$$(i) \text{ Rank } \frac{\partial \lambda}{\partial x}(x) = n, \forall x \in V \quad (ii) \lambda(x_0(\theta)) = x_0(\bar{\theta})$$

$$(iii) \text{ (PDE) } \left\{ \begin{array}{l} (1) f(\lambda(x), \bar{\theta}) = \frac{\partial \lambda}{\partial x}(x) f(x, \theta) \\ (2) g(\lambda(x), \bar{\theta}) = \frac{\partial \lambda}{\partial x}(x) g(x, \theta) \quad \text{for all } x \in V. \\ (3) h(\lambda(x), \bar{\theta}) = h(x, \theta) \end{array} \right.$$

Then there exists t_1 , $0 < t_1 < T$, such that $\Sigma_{x_0(\theta)}^\theta$ is globally identifiable at θ , in the sense of Definition 0.2 and with $u \in \mathcal{U}[0, t_1]$, if and only if (i), (ii), (iii) $\Rightarrow \theta = \bar{\theta}$.

Vajda et al. [17] treated some examples but did not give a systematic procedure to apply this theorem, which is stated in analytic terms. A new algorithm for analyzing identifiability, based on this theorem and the differential algebra theory, is presented here.

On the other hand, this approach is not valid for uncontrolled nonlinear dynamical systems as it has been proved in [11]. In this case, an efficient approach [5] gives identifiability results of some particular systems.

2.2 Symbolic computation procedure

Considering the derivation $\frac{\partial}{\partial x}$ the system (PDE) can be rewritten as a differential polynomial system that will be completed with

$$\frac{\partial \bar{\theta}_i}{\partial x_j} = 0, \quad i = 1, \dots, q, \quad j = 1, \dots, n. \quad (8)$$

The resulting system can be described by the following polynomial equations and inequations:

$$(pde) \left\{ \begin{array}{l} p(x, \bar{x}, \frac{\partial \bar{x}}{\partial x_1}, \dots, \frac{\partial \bar{x}}{\partial x_n}, \theta, \bar{\theta}) = 0 \\ q(x, \bar{x}, \theta, \bar{\theta}) = 0, \\ r(x, \bar{x}, \frac{\partial \bar{x}}{\partial x_1}, \dots, \frac{\partial \bar{x}}{\partial x_n}, \theta, \bar{\theta}) \neq 0 \\ \frac{\partial \bar{\theta}_i}{\partial x_j} = 0, i = 1, \dots, q, j = 1, \dots, n. \end{array} \right. \quad (9)$$

In this sub-section, \mathcal{I} will denote the radical of the ideal, generated by the equations of the system (9). It can be considered in the differential ring $K(\theta)\{x, \bar{x}, \bar{\theta}\}$. Once again, the pure transcendental field extension $K(\theta)$ is considered as a field of coefficients, which leads to a structural identifiability.

From the ranking $[\bar{\theta}] \prec [\bar{x}]$, a characteristic presentation of \mathcal{I} is computed.

Rosenfeld-Groebner algorithm cannot solve, in the analytic sense, system (PDE) stated in theorem (2.1). It computes integrability constraints by giving all the classes of solutions of the system. The relations between integrability constraints and parameter (un)identifiability are given in the propositions below.

Proposition 2.1 *If the radical of \mathcal{I} , endowed with the ranking $[\bar{\theta}] \prec [\bar{x}]$, admits a characteristic presentation, this characteristic presentation has the following form:*

$$\begin{aligned} &P_{1,1}(\bar{\theta}_1), \dots, P_{1,q_1}(\bar{\theta}_1), P_{2,1}(\bar{\theta}_1, \bar{\theta}_2), \dots, P_{2,q_2}(\bar{\theta}_1, \bar{\theta}_2), \dots, P_{q,1}(\bar{\theta}_1, \dots, \bar{\theta}_q), \\ &P_{q,2}(\bar{\theta}_1, \dots, \bar{\theta}_q), \dots, P_{q,q_q}(\bar{\theta}_1, \dots, \bar{\theta}_q), Q_{1,1}(\bar{\theta}, \bar{x}_1), \dots, Q_{1,n_1}(\bar{\theta}, \bar{x}_1), \\ &Q_{2,1}(\bar{\theta}, \bar{x}_1, \bar{x}_2), \dots, Q_{2,n_2}(\bar{\theta}, \bar{x}_1, \bar{x}_2), \dots, Q_{n,1}(\bar{\theta}, \bar{x}), \dots, Q_{n,n_n}(\bar{\theta}, \bar{x}), \end{aligned} \quad (10)$$

where $q_j \leq n$ for $j = 1, \dots, q$, $n_k \leq n$ for $k = 1, \dots, n$, the leader of the polynomial $P_{i,j}$ is a derivative of $\bar{\theta}_i$ and the leader of the polynomial $Q_{k,l}$ is a derivative of \bar{x}_k .

Proof - In the characteristic presentation \mathcal{C} , the polynomials $\frac{\partial \bar{\theta}_i}{\partial x_j}$ ($1 \leq i \leq q, 1 \leq j \leq n$) or lower ranked polynomials are found. Such polynomials admit $\frac{\partial \bar{\theta}_i}{\partial x_j}$ or $\bar{\theta}_i$ as leader. As \mathcal{C} is a differentially triangular set, the leaders of \mathcal{C} are different and its elements are reduced pairwise. As a consequence, in the characteristic presentation \mathcal{C} , there exists a maximum number of n polynomials whose leading variable is $\bar{\theta}_i$ for all $i = 1, \dots, q$.

In the same way, the existence of Q_{j,n_j} for $j = 1, \dots, n$ can be shown. \square

Admittedly it is impossible to know a priori the number of polynomials of the characteristic presentation.

Proposition 2.2 *The system $\Sigma_{x_0(\theta)}^\theta$ is assumed to be locally reduced at $x_0(\theta)$ for all $\theta \in \Omega_q$. The model is globally structurally identifiable in the sense of Definition 0.2 if \mathcal{I} endowed with the ranking $[\bar{\theta}] \prec [\bar{x}]$, admits a unique characteristic presentation which, moreover, has the following form*

$$\{\bar{x}_1 - x_1, \dots, \bar{x}_n - x_n, \bar{\theta}_1 - \theta_1, \dots, \bar{\theta}_q - \theta_q\}. \quad (11)$$

Proof - The assumption about the local reduction of $\Sigma_{x_0(\theta)}^\theta$ and the solution of the system (PDE) allow the application of Theorem 2.1. \square

Theorem 2.1 considers the analytic definition of identifiability, given in Definition 0.2. Thus, when the identifiability is not obtained directly (i.e. by ignoring initial conditions), a last calculation remains to be done: the evaluation of the equations of the characteristic presentation in $x_0(\bar{\theta})$. It selects the characteristic presentation valid for the particular initial conditions $x_0(\theta)$ and it examines if those initial conditions imply the unicity of the characteristic presentation.

Proposition 2.3 *The system $\Sigma_{x_0(\theta)}^\theta$ is assumed to be locally reduced at $x_0(\theta)$ for all $\theta \in \Omega_q$. The model is globally structurally identifiable in the sense of the definition 0.2 if and only if \mathcal{I} endowed with the ranking $[\bar{\theta}] \prec [\bar{x}]$, admits a unique characteristic presentation \mathcal{C} such that $\mathcal{C} = 0$, complete with $\lambda(x_0(\theta)) = x_0(\bar{\theta})$, implies $\{x = \bar{x}, \theta = \bar{\theta}\}$.*

Proof - Rosenfeld-Groebner algorithm returns k characteristic presentations $\mathcal{C}_1, \dots, \mathcal{C}_k$ of regular differential ideals $\mathcal{I}_1, \dots, \mathcal{I}_k$. These ideals correspond to different solution classes of the system (9). Now, since the model is globally identifiable, system (9) complete with $\lambda(x_0(\theta)) = x_0(\bar{\theta})$ ($\theta \in \Omega_q, \bar{\theta} \in \Omega_q$) has a unique solution $\{x = \bar{x}, \theta = \bar{\theta}\}$. Therefore, one and only one characteristic presentation \mathcal{C} among $\{\mathcal{C}_1, \dots, \mathcal{C}_k\}$ is compatible with $\lambda(x_0(\theta)) = x_0(\bar{\theta})$ ($\theta \in \Omega_q, \bar{\theta} \in \Omega_q$). Thus, the system $\mathcal{C} = 0$ complete with $\lambda(x_0(\theta)) = x_0(\bar{\theta})$ will give the same solution as system (PDE) complete with $\lambda(x_0(\theta)) = x_0(\bar{\theta})$, i.e. $\{x = \bar{x}, \theta = \bar{\theta}\}$.

The reciprocal is obvious. \square

2.3 Algorithm

The ensuing algorithm (denoted by **Algo2**) requires only the data of the functions f, g, h and $x_0(\theta)$. It is implemented in MAPLE VII. It is decomposed in three steps.

Step 1 This step tests the local reduction of the model $\Sigma_{x_0(\theta)}^\theta$ at $x_0(\theta)$ for all $\theta \in \Omega_q$ by using the observability rank criterion (ORC) and the controllability rank criterion (CRC) [16][9].

Step 2 This step corresponds to the differential algebraic treatment of system (PDE).

Firstly, it rewrites the system (PDE) as the system (9).

Secondly, the field of constants $K(\theta)$ and the ranking: $[\bar{\theta}] \prec [\bar{x}]$ are implicitly introduced.

Thirdly, integrability constraints are computed: Rosenfeld-Groebner algorithm computes the input-output characteristic presentations. If the software returns a unique characteristic presentation which, has the following form: $\{\bar{x} - x, \bar{\theta} - \theta\}$, then the model is structurally globally identifiable and the algorithm stops. Else the step 3 is considered.

Step 3 The equations of each characteristic presentation are evaluated in $x_0(\bar{\theta})$. It selects characteristic presentations valid for the particular initial conditions $x_0(\theta)$ and it examines if those initial conditions imply $\bar{\theta} = \theta$. Consequently identifiability results are given.

3 Examples

In this section, two examples are presented in order to illustrate both algorithms described above. The first one is academic and shows the importance of initial conditions in some controlled systems. The second one is a pharmacokinetic model for which identifiability does not require the knowledge of initial conditions. In this case, the first algorithm gives an exhaustive description of all the possible cases.

3.1 An academic example

The following *academic example* was treated without control in [5]:

$$\begin{cases} \dot{x}_1 &= \theta_1 x_1^2 + \theta_2 x_1 x_2 + u \\ \dot{x}_2 &= \theta_3 x_1^2 + \theta_4 x_1 x_2 \\ y &= x_1 \end{cases} \quad (12)$$

Here are the different steps of Algo1:

- *Step 1:* The software rewrites the system as :

$$\begin{cases} \dot{x}_1 &= \theta_1 x_1^2 + \theta_2 x_1 x_2 + u \\ \dot{x}_2 &= \theta_3 x_1^2 + \theta_4 x_1 x_2 \\ y &= x_1 \\ \dot{\theta} &= 0 \end{cases} \quad (13)$$

- *Step 2:* The SARC is satisfied if $\theta_3\theta_4 \neq 0$
- *Step 3:* The field of constants \mathbb{R} is chosen and the standard ranking is implicitly introduced.
- *Step 4:* Algo1 returns three cases:
 - i) The general case $\Omega_q = \{(\theta_1, \theta_2, \theta_3, \theta_4) \in \mathbb{R}^4, \theta_1\theta_2\theta_4 \neq 0\}$ is given by the input-output characteristic presentation:

$$\left\{ y\ddot{y} - y\dot{u} + y^2\theta_1\dot{y} + y^4\theta_2\theta_3 - uy - uy^2\theta_4 + \ddot{y}y^2 - y^4\theta_1\theta_4, \dot{\theta}_1, \dot{\theta}_2, \dot{\theta}_3, \dot{\theta}_4 \right\}. \quad (14)$$

- ii) $\theta_2 = 0$ is a particular case ($\Omega_q = \{(\theta_1, \theta_2, \theta_3, \theta_4) \in \mathbb{R}^4, \theta_2 = 0, \theta_1\theta_4 \neq 0\}$) corresponding to the input-output characteristic presentation:

$$\{-u + \dot{y} - y^2\theta_1, \dot{\theta}_1, \dot{\theta}_3, \dot{\theta}_4, \theta_2\}. \quad (15)$$

- iii) $y = 0$.

The general characteristic presentation i) is chosen.

- *Step 5:* the hypothesis of Proposition 1.2 is checked to be valid for all $\theta \in \Omega_q$.
- *Step 6:* The exhaustive summary given by the software is $(\theta_1, \theta_4, \theta_1\theta_4 - \theta_2\theta_3)$.
- *Step 7:* The analysis of this exhaustive summary leads to

$$\left\{ \bar{\theta}_1 - \theta_1, \bar{\theta}_2\bar{\theta}_3 - \theta_2\theta_3, \dot{\bar{\theta}}_3, \bar{\theta}_4 - \theta_4 \right\}. \quad (16)$$

which proves that the model is not globally identifiable at $\theta \in \Omega_q$.

Now the particular characteristic presentation ii) is chosen.

- *Step 5:* the hypothesis of Proposition 1.2 is checked to be valid for all $\theta \in \Omega_q$.
- *Step 6-7:* The exhaustive summary is: (θ_1) and its analysis leads to

$$\left\{ \bar{\theta}_1 - \theta_1, \dot{\bar{\theta}}_4, \dot{\bar{\theta}}_3, \dot{\bar{\theta}}_4 \right\}. \quad (17)$$

The model is not globally identifiable at $\theta \in \Omega_q$.

Finally the characteristic presentation iii) corresponds to a non generic solution

Algo2 is applied to the same example with the initial conditions $x_1(0) = x_2(0) = 0$.

- *Step 1:* the model is locally reduced at $(0,0)$ for every $\theta \in \{\theta \in \mathbb{R}^4, \theta_2\theta_3 \neq 0\}$.
- *Step 2:* It sets up the (PDE) system in the following form:

$$\begin{cases} \bar{\theta}_1 \bar{x}_1^2 + \bar{\theta}_2 \bar{x}_1 \bar{x}_2 = \lambda_1^1 (\theta_1 x_1^2 + \theta_2 x_1 x_2) + \lambda_2^1 (\theta_3 x_1^2 + \theta_4 x_1 x_2) \\ \bar{\theta}_3 \bar{x}_1^2 + \bar{\theta}_4 \bar{x}_1 \bar{x}_2 = \lambda_1^2 (\theta_1 x_1^2 + \theta_2 x_1 x_2) + \lambda_2^2 (\theta_3 x_1^2 + \theta_4 x_1 x_2) \\ 1 = \lambda_1^1 \\ 0 = \lambda_1^2 \\ \bar{x}_1 = x_1 \end{cases} \quad (18)$$

where $\bar{x} = \lambda(x)$ and $\lambda_j^i = \frac{\partial \lambda_i}{\partial x_j}$.

- *Step 3:* It returns only one characteristic presentation:

$$C = \left\{ \bar{x}_1 - x_1, \theta_3 \bar{x}_2 - x_2 \bar{\theta}_3, \frac{\partial \bar{\theta}_3}{\partial x_1}, \frac{\partial \bar{\theta}_3}{\partial x_2}, \theta_1 - \bar{\theta}_1, \theta_2 \theta_3 - \bar{\theta}_2 \bar{\theta}_3, \theta_4 - \bar{\theta}_4 \right\}. \quad (19)$$

The characteristic presentation is not enough to decide on the identifiability. The initial conditions have to be taken into account. Thus, according to Proposition 2.3, the equality $\lambda(0, 0) = (0, 0)$ is added to $C = 0$. No extra information is deduced; consequently the model is not structurally globally identifiable.

Then **Algo2** is applied to the same example with the initial conditions $x_1(0) = 0, x_2(0) = 1$.

- *Step 1*: the model is locally reduced at $(0, 1)$ for every $\theta \in \{\theta \in \mathbb{R}^4, \theta_2\theta_4 \neq 0\}$.
- *Step 2*: It is unchanged.
- *Step 3*: Equations $C = 0$ complete with $\lambda(0, 1) = (0, 1)$, lead to

$$\theta_3 = \bar{\theta}_3, \theta_2 = \bar{\theta}_2, \theta_4 = \bar{\theta}_4, \theta_1 = \bar{\theta}_1.$$

Therefore the model is structurally globally identifiable.

In this case, the structural global identifiability of the model is due to the initial conditions. This is a particular interest of Algo2: it takes the initial conditions into account easily while Algo1 does not do it. Moreover it is possible to complete Algo1 if initial conditions are known by evaluating the equations of the characteristic presentation at $t = 0$ and examining if they imply the unicity of parameters. It is the method chosen in [1] with characteristic presentation replaced by characteristic set. In the case $x_0 = (0, 1)$ the evaluation of the characteristic presentation, given by Algo1 in x_0 , does not give any answers. Therefore Algo2 is more efficient for this particular case.

3.2 A real pharmacokinetic model

Now a real pharmacokinetic model [4] is considered. It was solved by pen and paper in [10]:

$$\begin{cases} \dot{x}_1 &= \alpha_1(x_2 - x_1) - \frac{V_m x_1}{k_c + x_1} + u(t) \\ \dot{x}_2 &= \alpha_2(x_1 - x_2) \\ y &= x_1 \end{cases} \quad (20)$$

The unknown vector parameter is $\theta = \{\alpha_1, \alpha_2, k_c, V_m\}$. Here are the different steps of **Algo1**:

- *Step 1*: The software rewrites the system as the following polynomial differential system:

$$\begin{cases} \dot{x}_1(k_c + x_1) &= \alpha_1(x_2 - x_1)(k_c + x_1) - (V_m x_1) + u(t)(k_c + x_1) \\ \dot{x}_2 &= \alpha_2(x_1 - x_2) \\ y &= x_1 \\ k_c + x_1 &\neq 0 \end{cases} \quad (21)$$

- *Step 2*: The SARC is satisfied if $\alpha_2 \neq 0$.
- *Step 3*: The field of constants \mathbb{R} is chosen and the standard ranking is implicitly introduced.
- *Step 4*: Algo1 returns two cases:

- The general case $\Omega_q = \{\theta \in \mathbb{R}^4, \alpha_1 \neq 0\}$ is given by the input-output characteristic presentation:

$$\{2k_c \ddot{y} + k_c^2 \dot{y} + (\alpha_1 + \alpha_2) \dot{y} y^2 + 2k_c(\alpha_1 + \alpha_2) \dot{y} y + ((\alpha_1 + \alpha_2)k_c + V_m)k_c \dot{y} + \alpha_2 V_m y^2 + \alpha_2 V_m k_c y - u \alpha_2 k_c^2 - \alpha_2 u y^2 - 2k_c y \dot{u} - \dot{u} y^2 - k_c^2 \dot{u} - 2\alpha_2 k_c u y - \ddot{y} y^2, \dot{\alpha}_1, \dot{\alpha}_2, \dot{V}_m, \dot{k}_c\}. \quad (22)$$

- $\alpha_1 = 0$ is a particular case ($\Omega_q = \{\theta \in \mathbb{R}^4, \alpha_1 = 0\}$) presented by the input-output characteristic presentation:

$$\{ \dot{y}(k_c + y) + V_m y - u k_c - u y, \alpha_1, \dot{\alpha}_2, \dot{V}_m, \dot{k}_c \}. \quad (23)$$

The general characteristic presentation is chosen.

- *Step 5:* The hypothesis of Proposition 1.2 is not valid if $V_m k_c = 0$. Indeed, the set L is reduced to $L = \{\dot{y}\}$ and the input-output characteristic presentation can be rewritten as

$$\{(y + k_c)^2 \dot{y} + T, \dot{\alpha}_1, \dot{\alpha}_2, \dot{V}_m, \dot{k}_c\}$$

where $(y + k_c)^2$ and T belong to $\mathbb{R}[N]$. If $V_m = 0$, $(y + k_c)^2$ is a divisor of T and if $k_c = 0$, y^2 is a divisor of T . Consequently, the set Ω_q becomes $\Omega_q = \{\theta \in \mathbb{R}^4, \alpha_1 = 0, V_m k_c \neq 0\}$.

- *Step 6:* The exhaustive summary, given by the software, is :

$$(-k_c^2 \alpha_2, k_c \alpha_2 V_m, -k_c^2, k_c \alpha_2, k_c, -\alpha_2, -k_c, k_c(\alpha_1 + \alpha_2), \alpha_1 + \alpha_2, -k_c(k_c \alpha_2 + k_c \alpha_1 + V_m)) \quad (24)$$

- *Step 7:* The analysis of this exhaustive summary leads to :

$$\{V_m - \bar{V}_m, k_c - \bar{k}_c, \alpha_1 - \bar{\alpha}_1, \alpha_2 - \bar{\alpha}_2\} \quad (25)$$

which proves that the model is structurally globally identifiable.

Now the particular characteristic presentation *ii)* is chosen.

- *Step 5:* The hypothesis of Proposition 1.2 is not valid if $V_m k_c = 0$. Therefore $\Omega_q = \{\theta \in \mathbb{R}^4, \alpha_1 = 0, V_m k_c \neq 0\}$.
- *Step 6-7:* The exhaustive summary is: $(V_m, k_c, -k_c)$ and its analysis leads to

$$\{\bar{V}_m - V_m, \bar{k}_c - k_c, \dot{\alpha}_1, \dot{\alpha}_2\}. \quad (26)$$

The model is not globally identifiable at $\theta \in \Omega_q$.

Algo2 is applied to the same example with initial conditions $x_1(0) = 0, x_2(0) = 0$.

- *Step 1:* The algorithm shows that the model is not locally reduced at $(0, 0)$ if $\alpha_1 \alpha_2 = 0$.
- *Step 2:* After writing the (PDE) system, the algorithm gives a unique characteristic presentation containing:

$$\{\bar{x}_1 - x_1, \bar{x}_2 - x_2, V_m - \bar{V}_m, k_c - \bar{k}_c, \alpha_1 - \bar{\alpha}_1, \alpha_2 - \bar{\alpha}_2\}.$$

Therefore the model is structurally globally identifiable. The algorithm stops: step 3 is useless.

The cases $V_m = 0$ and $k_c = 0$ do not appear explicitly since the pure transcendental field extension $K(\theta)$ is considered as the field of coefficients in all the algorithm.

Therefore, results of Algo2 agree with results of Algo1 but the analysis is less exhaustive.

3.3 Comparison of algorithms

Algo1 is well adapted for an exhaustive analysis of the global identifiability of a model independently on initial conditions. On the other hand, as shown in the case of the academic example, Algo2 is efficient if initial conditions are a significant part of the model.

It is possible to compare algorithm efficiency relatively to the computation time on a pentium 4 with 2.2 MHz.

- example (12) - 1s (Algo1), 1.2s (Algo2),
- example (20) - 1.1s (Algo1), 1.3s (Algo2)

Then Algo1 is slightly faster than Algo2. Moreover some examples, not given here, show that Algo2 may fail more easily when the dimension of the model is too large.

The authors put the software at the disposal of anyone concerned by this kind of problem.

4 Conclusion

In this paper, we have shown how to analyze algorithmically the identifiability of nonlinear controlled dynamical models from two different approaches.

The input-output approach does not make use of initial conditions but can be applied also to systems given in implicit form or to uncontrolled models. The concept of characteristic presentations of the input-output ideal permits the elaboration of an algorithm such that all the steps are computed by software. Moreover, the computation of characteristic presentations point out particular cases whose exhaustive analysis is done by the algorithm.

The similarity transformation approach considers initial conditions which are well defined after selecting parameter values. It requires the local reduction at initial conditions; it is tested easily by the first step of the algorithm. This approach leads to the solution of a PDE system. Some results concerning the characteristic presentation of the ideal, generated by this PDE system, permit the elaboration of the steps concerning identifiability analysis. However, it is not possible to obtain identifiability properties for the parameter values corresponding to loss of reduction.

In conclusion, both of them have been applied successfully to different models. But, although tested efficiently on some significant models, there is still much room for algorithmic improvements.

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