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An efficient algorithm for testing nonlinear dynamical model identifiability

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Abstract

This paper is concerned by the analysis of nonlinear controlled or uncontrolled dynamical model identifiability. The proposed approach is based on the construction of an input-output ideal. The aim is to develop an algorithm which gives identifiability results from this approach. Differential algebra theory allows realization of such a project. In order to state the algorithm, new results of differential algebra must be proved. Then the implementation is done in a symbolic computing language.

Introduction

In this paper, the following model is introduced in order to analyze nonlinear controlled or uncontrolled dynamical model identifiability.

The initial conditions are ignored:

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

In this model, $x(t, \theta) \in \mathbb{R}^n$, $y(t, \theta) \in \mathbb{R}^m$, $u(t) \in \mathbb{R}$ denote the state variables, the measured outputs, and the input respectively. The parameter vector θ is in Ω_q , a subset of \mathbb{R}^q (or C^q). The single-input case is taken into account for notational simplicity; all the results can be generalized readily. What follows is developed in the case of controlled models and can be applied easily if models are uncontrolled ($u = 0$). The functions $f(x, \theta)$, $g(x, \theta)$ and $h(x, \theta)$ are rational and may depend on a known constant vector denoted by a .

In the 90's Diop and Fliess [7], Fliess and Glad [9], Ljung and Glad [14] and Ollivier [16] proposed a new approach for identifiability, based on differential algebra. Following this idea, we have elaborated an algorithm for analyzing identifiability, which requires some knowledge of differential algebra theory.

Now, let us introduce some useful notations (see also Appendix B).

- 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 differential 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 $\Theta\tilde{V}$).

Here, the field of constants is $\mathbb{R}(a)$ (i.e. the field generated by \mathbb{R} and a) if the functions $f(x, \theta)$, $g(x, \theta)$ and $h(x, \theta)$ depend on a , otherwise it is \mathbb{R} . Then the differential field K is defined as the field of constants equipped with the derivation $\frac{d}{dt}$.

Indeed, the model Σ^θ is considered as a set of variables $\{u, x, y, \theta\}$ linked by a differential ideal. More precisely it can be rewritten as a differential polynomial model completed with $\dot{\theta}_i = 0, i = 1, \dots, q$. The resulting system Γ can be described by the following polynomial equations and inequations.

$$\Gamma \begin{cases} p(\dot{x}, x, u, \theta) = 0, \\ q(x, y, \theta) = 0, \\ \dot{\theta}_i = 0, i = 1, \dots, q \\ r(x, y, \theta) \neq 0. \end{cases} \quad (2)$$

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

These models are very general. Thus, the solutions of the system may be non-unique and some solutions might be of a degenerate character. Therefore, the concept of non-degenerate solutions [14] have to be considered. In the following the definitions introduced in [7] are adopted:

Definition 0.1 *A model is algebraically identifiable if and only if any parameter θ_i is algebraic over $K\langle u, y \rangle$.*

This definition is strongly connected to the nonlinear observability.

Definition 0.2

A model is rationally identifiable if and only if any parameter θ_i belongs to the field $K\langle u, y \rangle$.

Ljung and Glad [14] and Ollivier [16] exploited the concept of characteristic set. The characteristic set of the differential ideal, defined by dynamical model equations, is a finite set of polynomials which summarises the whole information contained in the differential ideal (see Appendix C). 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. 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 by analyzing the characteristic set. This last analysis is done by Audoly et al ([1]) by using Groebner basis calculation. They have chosen numerical random points rather than symbolic points to enlarge the class of models testable by their algorithm.

In the 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 (see Appendix C for more details) The identifiability is obtained after analyzing the characteristic presentation using symbolic points rather than numerical random points and the suggested method allows the analysis of a class of models that is as large as in [1]. The resulting algorithm is only based on differential algebra. It is implemented in MAPLE, a symbolic computation language, and uses the package DIFFALG especially.

The paper is organized as follows. First, section 1 proves some results necessary to the development of the identifiability algorithm. Section 2 gives results of identifiability in the most general framework. Section 3 considers $K(\theta)$ instead of K , which allows a significant simplification of the algorithm while giving general identifiability results. Then section 4 describes the algorithm and its features. Finally, the algorithm is used for analyzing identifiability of some nonlinear academic, pharmacokinetic and physiological models and its efficiency is pointed out.

In our approach, differential algebra allows the validation of the proposed algorithm. If the reader is unfamiliar with such notions [13], some useful definitions and propositions can be found in Appendices A, B and C.

1 Characteristic presentation

The differential ideal generated by the equations of Γ is considered in the differential field $K\langle x, y, u, \theta \rangle$. Its radical is denoted by \mathcal{I} . From the ranking:

$$[\theta] \prec [y, u] \prec [x] \quad (3)$$

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

Proposition 1.1 *If \mathcal{I} , endowed with the ranking (3), admits a characteristic presentation, this presentation has the following form:*

$$\{\dot{\theta}_1, \dots, \dot{\theta}_q, P_1(y, u, \theta), \dots, P_m(y, u, \theta), Q_1(y, u, \theta, x), \dots, Q_n(y, u, \theta, x)\} \quad (4)$$

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 $j = 1, \dots, n$.

Proof - We propose to the reader unfamiliar with differential algebra to consult Appendices B and C, necessary to the proof understanding.

Let \mathcal{C} be a characteristic presentation of \mathcal{I} .

- In a first time, we prove that *the differential polynomials $\dot{\theta}_i$, $i = 1, \dots, q$ are in \mathcal{C}* :

θ_i has a minimal ranking in (3) so only differential polynomials which have $\dot{\theta}_i$, or a lower ranked variable as leader, are in \mathcal{C} . Such a polynomial is written $\theta_i + W$, with $W \in K\langle \theta_1, \dots, \theta_{i-1} \rangle$. If such a polynomial exists, it lies in the ideal \mathcal{I} and, by definition, it will be rewritten as zero modulo the rewriting rules of every characteristic presentation of this ideal, corresponding to different rankings. If the ranking $[\theta] \prec [u] \prec [x] \prec [y]$ is considered, the set of the polynomials involved in Γ consists in the characteristic presentation of \mathcal{I} (only implicit models are considered). However, no polynomial of Γ admits θ_i as leader. Therefore, if $W \neq 0$, the rewriting rules cannot rewrite as zero the differential polynomial $\theta_i + W$. Finally, $\theta_i + W$ does not lie in \mathcal{I} . Therefore, for $i = 1, \dots, q$, $\dot{\theta}_i \in \mathcal{C}$.

- In the same way, one can prove that *\mathcal{C} does not contain any polynomial of the form $F(u, \theta)$.*
- Now we show that *there exists a unique polynomial, in \mathcal{C} , of the form $P_i(y, u, \theta)$ whose y_i is the leading variable, for all $i = 1, \dots, m$:*

Since y_i is differentially algebraic over $K\langle u, \theta \rangle$, for all $i = 1, \dots, m$, there exist some polynomials of the form $P_i(y, u, \theta)$ in \mathcal{I} . Let us suppose that y_i is not the leading variable of any element of \mathcal{C} and let us consider the polynomials of \mathcal{C} which have a leader lower than $P_i(y, u, \theta)$. B is the set containing such elements. As it is a subset of a differentially triangular set, B is also a differentially triangular set. A differentially triangular set lower than B is created by placing $P_i(y, u, \theta)$, or its partial remainder w.r.t the polynomials $P_k(y, u, \theta)$ ($1 \leq k < i$), as the last polynomial in B . The other elements of \mathcal{C} are partially reduced w.r.t this added polynomial in order to obtain a differentially triangular set lower than \mathcal{C} . But \mathcal{C} is minimal by hypothesis. This contradiction implies that y_i is the leading variable of a polynomial of \mathcal{C} for all $i = 1, \dots, m$. As in ordinary differential algebra, the polynomials of a triangular set have different principal variables, so there exists exactly the quantity m of such polynomials.

- In the same way, *the existence of exactly n polynomials of the form $Q(y, u, \theta, x)$ can be proved.* \square

In general, \mathcal{I} should be written as the intersection of regular differential ideals, each one admitting a characteristic presentation (see (34) in Appendix D). However in the following, \mathcal{I} , endowed with the ranking (3), 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:

- $\mathcal{C}(\theta)$ 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 $[y, u] \prec [x]$.

In order 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 (3).

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 $\theta \in \Omega_q$.

Proof - In this proposition the set of the leaders L of the elements of \mathcal{C} is considered, N denotes the other derivatives occurring in \mathcal{C} and $K[N]$ is the polynomial ring built over N with coefficients in K .

This proof uses the results and the notations of Appendix C.

Let us notice that \mathcal{C} is strongly normalized. Thus, each initial of \mathcal{C} is in $K[N]$, and θ_i cannot be the leader of any polynomial in \mathcal{C} (see [15]). $\mathcal{C}(\theta)$ is a characteristic set since it satisfies the two following points:

- $\mathcal{C}(\theta)$ is an autoreduced set since the evaluation of the polynomials c_i remains the leader (θ has been assumed not to cancel initials). Moreover, such an evaluation does not change the degree of elements of L appearing in the polynomials c_i .
- Suppose that there exists a polynomial p reduced w.r.t $\mathcal{C}(\theta)$. Such a polynomial is reduced w.r.t \mathcal{C} and, since \mathcal{C} is a characteristic set of \mathcal{I} , $p = 0$.

Next, the evaluation in θ does not change the leaders of any polynomial of \mathcal{C} . Since \mathcal{C} is strongly normalized, $\mathcal{C}(\theta)$ is also strongly normalized. The elements of $\mathcal{C}(\theta)$ are primitive on $K[N]$ because, by assumption, the evaluated coefficients have no common factor.

In this way, $\mathcal{C}(\theta)$ is a characteristic presentation of \mathcal{I}_θ . Therefore the uniqueness of the characteristic presentation of an ideal, endowed with a ranking, implies $\mathcal{C}_\theta = \mathcal{C}(\theta)$. \square

2 Input-output ideal and identifiability results

Now let us introduce \mathcal{I}_θ^{io} , the ideal obtained after eliminating state variables. Thus the set $\mathcal{C}_\theta^{io} = \mathcal{C}_\theta \cap K(\theta)\{u, y\}$ 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 polynomials $P_i, i = 1 \dots m$, of \mathcal{C}_θ^{io} can be seen as polynomials in y, u and their derivatives with coefficients in $K(\theta)$. In the following, those polynomials will be written as

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

where m_0^i is not equal to zero. Let us denote by d_i for $i = 1 \dots m$, the Wronskians of functions $m_k^i(y, u), k = 1 \dots n_i$. The non-degenerate solution, evocated in the introduction, is defined by:

Definition 2.1 A non-degenerate solution (x, y, u, θ) of Γ is a solution such that

- (i) no separant or initial of P_i ($i = 1 \dots m$) and Q_j ($j = 1 \dots n$) in (4) is zero,
- (ii) no Wronskian d_i ($i = 1 \dots m$) is zero.

2.1 Rational identifiability and input-output characteristic presentation

In this section, we assume $\mathcal{C}_\theta = \mathcal{C}(\theta)$ for all θ .

Proposition 2.1 Let θ and $\bar{\theta}$ two parameter vectors and \mathcal{C}_θ^{io} and $\mathcal{C}_{\bar{\theta}}^{io}$ the corresponding input-output characteristic presentations. The corresponding solutions of Γ are assumed to be respectively (x, y, u, θ) and $(\bar{x}, y, u, \bar{\theta})$ and non-degenerate solutions. Then

$$\forall \bar{\theta} \in \Omega_q \quad \mathcal{C}_\theta^{io} = \mathcal{C}_{\bar{\theta}}^{io} \Rightarrow (p_k^i(\theta) = p_k^i(\bar{\theta}), k = 1 \dots n_i, i = 1 \dots m).$$

Proof - It is clear that $\mathcal{C}_\theta^{io} = \mathcal{C}_{\bar{\theta}}^{io}$ is equivalent to $P_i(y, u, \theta) = P_i(y, u, \bar{\theta}), i = 1 \dots m$ for all y and u (the set of polynomials $P_i(y, u, \theta)$ is a triangular set). Since (y, u) satisfy (ii) (definition 2.1), the previous equalities imply the equalities of the coefficients of the functions $m_k^i(y, u), k = 1 \dots n_i, i = 1 \dots m$. \square

Remark 2.1 Moreover, under the assumptions of the previous proposition, it is easy to prove that $p_k^i(\theta)$ for $k = 1 \dots n_i, i = 1 \dots m$ are in the field $K \langle u, y \rangle$. Therefore, they will be rewritten as: $p_k^i(\theta) = g_k^i(y, u)$ ($k = 1 \dots n_i, i = 1 \dots m$).

2.2 Exhaustive summary and identifiability results

The *exhaustive summary* [20] of Γ is given by the vector of coefficients in θ :

$$\{p_k^i(\theta), k = 1 \dots n_i, i = 1 \dots m\}.$$

In order to deduce identifiability results from the exhaustive summary, the following system is considered:

$$p_k^i(\theta) = p_k^i(\bar{\theta}), k = 1, \dots, n_i, i = 1, \dots, m. \quad (5)$$

It can be rewritten as a differential polynomial system:

$$\mathcal{S}_u \begin{cases} p(\theta, \bar{\theta}) = 0, \\ \dot{\theta}_i = 0, i = 1, \dots, q, \\ \dot{\bar{\theta}}_i = 0, i = 1, \dots, q. \end{cases} \quad (6)$$

Let us denote by \mathcal{S} , the radical of the differential ideal generated \mathcal{S}_u , which is considered in $K \langle \theta, \bar{\theta} \rangle$ such that all particular cases are obtained.

Proposition 2.2 *If \mathcal{S} , endowed with the ranking $[\theta] \prec [\bar{\theta}]$, admits a characteristic presentation \mathcal{C} , \mathcal{C} has the following form:*

$$A_1(\theta_1), A_1(\theta_1, \theta_2), \dots, A_q(\theta_1, \dots, \theta_q), B_1(\theta, \bar{\theta}_1), B_2(\theta, \bar{\theta}_1, \bar{\theta}_2), \dots, B_q(\theta, \bar{\theta}_1, \dots, \bar{\theta}_q) \quad (7)$$

where the leader of the polynomial A_k is θ_k or $\dot{\theta}_k$ for $k = 1, \dots, q$, and where the leader of the polynomial B_j is $\bar{\theta}_j$ or $\dot{\bar{\theta}}_j$ for $j = 1, \dots, q$.

Proof - The functions $\dot{\theta}_i$ are in \mathcal{S} and θ_i has a minimal ranking in (3) so differential polynomials which have $\dot{\theta}_i$, or a lower ranked variable as leader, are in \mathcal{C} . 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 number of q polynomials whose leading variable is θ_i for all $i = 1, \dots, q$. In the same way, the existence of B_j ($j = 1, \dots, q$) can be shown. \square

In general, \mathcal{S} should be written as the intersection of regular differential ideals which admit a characteristic presentation (see (34) in Appendix D): a general component and particular components of the decomposition of the ideal. The particular components correspond to particular values of $(\theta, \bar{\theta})$ which are such that some separants or initials of (7) of the general component are equal to zero.

Proposition 2.3 *Let us assume that all separants and initials of polynomials in \mathcal{C} are non-zero. Then three different situations can arise in (7):*

- (i) All B_i are of order 0 and degree 1 in $\bar{\theta}_i$, and moreover $B_i = \bar{\theta}_i - \theta_i$.
- (ii) All B_i are of order 0 in $\bar{\theta}_i$, and some B_j is of degree > 1 in $\bar{\theta}_j$.
- (iii) For some i one has $B_i = \dot{\bar{\theta}}_i$.

Proof - This proposition is obvious. Let us only prove that $B_i = \bar{\theta}_i - \theta_i$ in the case (i). If each B_i is of degree one in $\bar{\theta}_i$, then it must be independant of the other $\bar{\theta}_j$ for (7) to be autoreduced (see appendices B and C). Thus each B_i can be rewritten as $P_i(\theta)\bar{\theta}_i - Q_i(\theta)$, where P_i and Q_i are polynomials. Then, the assumption of the proposition implies (6) to have one and only one solution. On the other hand $\theta = \bar{\theta}$ is a solution of (6) and the polynomials B_i are primitive over $K[\theta]$ (see appendix C and [3]), which leads to $B_i = \bar{\theta}_i - \theta_i$. \square

It leads to the following identifiability theorem.

Theorem 2.1 *Let us assume that all separants and initials of polynomials in \mathcal{C} are non-zero and that there exists a non-degenerate solution of Γ . If the characteristic presentation (7) has the form of*

- case (i) above, then the model is rationally identifiable.
- case (ii) above, then the model is algebraically identifiable.
- case (iii) above, then the model is not algebraically identifiable.

Proof - As seen in Remark 2.1, the elements of the exhaustive summary can be rewritten as:

$$p_k^i(\theta) = g_k^i(y, u), \quad k = 1 \dots n_i, i = 1 \dots m.$$

Moreover $g_k^i(y, u)$ is a differential rational function in y and u which is constant for $k = 1 \dots n_i, i = 1 \dots m$, and will be only denoted by g_k^i for $k = 1 \dots n_i, i = 1 \dots m$. Thus the system (5) can be rewritten:

$$\begin{cases} n_k^i(\bar{\theta}) = d_k^i(\bar{\theta})g_k^i, & k = 1, \dots, n_i, i = 1, \dots, m, \\ \bar{\theta}_i = 0, & i = 1, \dots, q, \\ \dot{g}_k^i = 0, & k = 1, \dots, n_i, i = 1, \dots, m, \end{cases} \quad (8)$$

where $n_k^i(\bar{\theta})$ and $d_k^i(\bar{\theta})$ are polynomials in $\bar{\theta}$. Then, it is easy to prove as previously that the differential ideal generated by (8) with the ranking

$$[g] \prec [\bar{\theta}], \quad (g = \{g_k^i, k = 1 \dots n_i, i = 1 \dots m\}) \quad (9)$$

admits a general characteristic presentation which contains the polynomials:

$$\{S_1(g, \bar{\theta}_1), S_2(g, \bar{\theta}_1, \bar{\theta}_2), \dots, S_q(g, \bar{\theta}_1, \dots, \bar{\theta}_q)\}. \quad (10)$$

The system (8) admits the same number of solutions as the system (6). Thus the polynomials S_i will be in the same situation as the polynomials B_i with regard to the order and the degree in $\bar{\theta}_i$. Since the $(g_k^i, k = 1 \dots n_i, i = 1 \dots m)$ are differential rational functions in y and u the results of the theorem 2.1 are deduced. \square

In the previous theorem, the most general results are obtained in taking the characteristic presentation of the general component. But all particular components can be analyzed by the same way, which leads to identifiability results of models corresponding to particular parameter values.

3 A simplified analysis with $K(\theta)$

When the particular cases are not interesting for the user, the components of θ can be assumed transcendent on K . The system Σ^θ can be rewritten:

$$\Gamma_\theta \begin{cases} p(\dot{x}, x, u, \theta) = 0, \\ q(x, y, \theta) = 0, \\ r(x, y, \theta) \neq 0, \end{cases} \quad (11)$$

and the differential ideal generated by the equations of Γ_θ can be considered in the differential field $K(\theta) \langle x, y, u \rangle$, where $K(\theta)$ corresponds to the field of constants $\mathbb{R}(a, \theta)$ or $\mathbb{R}(\theta)$. In this context, a solution of Γ_θ is a triplet of functions (x, y, u) satisfying all the model equations. The advantage of the choice of $K(\theta)$ is relative to the number and complexity of reductions which are consequently simplified, even if some particular cases are lost.

In this case \mathcal{J} denotes the radical of the differential ideal generated by the equations of Γ_θ with the ranking $[y, u] \prec [x]$. In the same way as in Proposition 1.1 if \mathcal{J} admits a characteristic presentation, it can be shown that this presentation has the following form:

$$\{P_1(y, u, \theta), \dots, P_m(y, u, \theta), Q_1(y, u, \theta, x), \dots, Q_n(y, u, \theta, x)\} \quad (12)$$

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 the following \mathcal{J} , endowed with the above ranking, is assumed to be a regular ideal presented by a characteristic presentation. In the opposite case, only the most general component will be considered. The input-output ideal and its characteristic presentation are defined the way it is done in the first section.

Definition 3.1 A non-degenerate solution (x, y, u) of Γ_θ is a solution such that
(i) no separant or initial of P_i ($i = 1 \dots m$) and Q_j ($j = 1 \dots n$) in (12) is equal to zero,
(ii) no Wronskian d_i ($i = 1 \dots m$) is zero.

Furthermore, the ideals \mathcal{I} (defined in section 1) and \mathcal{J} admit characteristic presentations which contain the same polynomials

$$\{P_1(y, u, \theta), \dots, P_m(y, u, \theta), Q_1(y, u, \theta, x), \dots, Q_n(y, u, \theta, x)\}. \quad (13)$$

Therefore Proposition 2.1 is also true.

The analysis of the exhaustive summary can be also simplified because each component θ_i is assumed to be transcendent on \mathbf{R} . The following differential polynomial system is considered:

$$S_\theta \left\{ \begin{array}{l} p(\theta, \bar{\theta}) = 0, \\ \dot{\bar{\theta}}_i = 0, i = 1, \dots, q. \end{array} \right. \quad (14)$$

The differential ideal generated by S_θ can be considered in the differential field $K(\theta) \langle \bar{\theta} \rangle$ to reduce the number and complexity of reductions. Let us denote \mathcal{S}_t the radical of the differential ideal generated by the equations of the system S_θ . With the ranking

$$[\bar{\theta}_1] \prec [\bar{\theta}_2] \prec [\dots] \prec [\bar{\theta}_q] \quad (15)$$

a characteristic presentation of \mathcal{S}_t is computed and it is easy to prove that this presentation has the following form:

$$\{B_1(\theta, \bar{\theta}_1), B_2(\theta, \bar{\theta}_1, \bar{\theta}_2), \dots, B_q(\theta, \bar{\theta}_1, \dots, \bar{\theta}_q)\} \quad (16)$$

where the leader of the polynomial B_j is $\bar{\theta}_j$ or $\dot{\bar{\theta}}_j$ for $j = 1, \dots, q$.

Here the general components of \mathcal{S} and \mathcal{S}_t contain the same polynomials (16).

Finally by this way Proposition 2.3 and Theorem 2.1 are also true if $K(\theta)$ is considered instead of K .

4 Algorithm

Now let us present the algorithm. It will be referred to it as **Algo**. Let us remark steps 3 and 7 of Algo1 are based on Rosenfeld-Groebner algorithm which has been realized by F. Boulier in MAPLE VII [2]. The algorithm is implemented in MAPLE VII and runs on any Pentium PC.

Data: f , g and h .

Step 1 The software rewrites the original system Σ^θ as the system Γ_θ defined by (2).

Step 2 The differential field K (or $K(\theta)$) 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 3 Rosenfeld-Groebner algorithm computes input-output characteristic presentations. If the differential field is $K(\theta)$ the general input-output characteristic presentation is only computed and the algorithm goes to step 5, otherwise an input-output characteristic presentation is chosen by the user.

Step 4 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 5 It verifies that the Wronskians d_i are not in the differential ideal generated by the equations of Γ (or Γ_θ).

Step 6 It saves the coefficients $p_k^i(\theta)$ in a list called the "exhaustive summary". This summary 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-Grobner algorithm: it is a purely differential and algebraic step. Then the results of identifiability are provided.

In this step the considered equations are symmetrical in θ and $\bar{\theta}$, which leads to a simplified reduction procedure. A priori, the analysis of the exhaustive summary leads to equations of the following type:

$$p_k^i(\theta) = g_k^i \text{ for } k = 1 \dots n_i, i = 1 \dots m, \quad (17)$$

which corresponds to $q + n_1 + \dots + n_m$ indeterminates and K is the differential field necessarily. Our strategy consists in rewriting the system such that it is symmetrical in θ and $\bar{\theta}$. In this case there are $2q$ indeterminates (often $2q \leq q + n_1 + \dots + n_m$). Moreover it is possible to chose $K(\theta)$ as differential field as in (14), which gives q indeterminates only. Consequently the number of indeterminates is significantly reduced.

Finally, let us note that if the algorithm does not successfully terminate because the computation of the input-output characteristic presentation is too complex or the analysis of the exhaustive summary fails, the algorithm can be reapplied by using a different ranking between the variables in steps 2 or (and) 7.

5 Examples

In this section, two examples are presented in order to illustrate the algorithm described above. The second one is a pharmaco-kinetic model . In each case, the algorithm gives an exhaustive description of all the possible cases.

5.1 An academic example

The following *academic example* was treated without control in [6]:

$$\begin{cases} \dot{x}_1 &= \theta_1 x_1^2 + \theta_2 x_1 x_2 + u \\ \dot{x}_2 &= \theta_3 x_1^2 + \theta_4 x_1 x_2 \\ y &= x_1 \end{cases} \quad (18)$$

Here are the different steps of **Algo**:

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

$$\begin{cases} \dot{x}_1 &= \theta_1 x_1^2 + \theta_2 x_1 x_2 + u \\ \dot{x}_2 &= \theta_3 x_1^2 + \theta_4 x_1 x_2 \\ y &= x_1 \\ \dot{\theta} &= 0 \end{cases} \quad (19)$$

- *Step 2*: The field of constants \mathbb{R} is chosen and the standard ranking is implicitly given.
- *Step 3*: **Algo** returns three cases:

- The general case ($\Omega_q = \{(\theta_1, \theta_2, \theta_3, \theta_4) \in \mathbb{R}^4, \theta_2 \neq 0\}$) is given by the following characteristic presentation:

$$\{x_1 - y, x_2 \theta_2 y^2 + y(-\dot{y} + y^2 \theta_1 + u), y\dot{y} + uy - y\dot{u} - \dot{y}^2 + uy^2 \theta_4 - (\theta_1 + \theta_4)\dot{y}y^2 - (\theta_2 \theta_3 - \theta_1 \theta_4)y^4, \dot{\theta}_1, \dot{\theta}_2, \dot{\theta}_3, \dot{\theta}_4\} \quad (20)$$

- $\theta_2 = 0$ (then $\Omega_q = \{(\theta_1, \theta_3, \theta_4) \in \mathbb{R}^3\}$) is a particular case corresponding to the characteristic presentation:

$$\{\dot{x}_2 - \theta_3 y^2 - \theta_4 y x_2, x_1 - y, -u + \dot{y} - y^2 \theta_1, \dot{\theta}_1, \dot{\theta}_3, \dot{\theta}_4, \theta_2\}. \quad (21)$$

- $y = 0$.

The characteristic presentation 20 corresponding to the case i) is chosen.

- *Step 4*: It verifies that the hypothesis of Proposition 1.2 is valid for all $\theta \in \Omega_q$.
- *Step 5*: It verifies that the Wronskian of $\{y^2\dot{y}, y^4, -uy^2\}$ is not equal to zero.
- *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

$$\{\bar{\theta}_1 - \theta_1, \bar{\theta}_2\bar{\theta}_3 - \theta_2\theta_3, \dot{\bar{\theta}}_3, \bar{\theta}_4 - \theta_4\}. \quad (22)$$

Thus θ_1, θ_4 and $\theta_2\theta_3$ are in the field $K\langle u, y \rangle$. But the analysis of this exhaustive summary proves that the model is not algebraically identifiable.

Now the characteristic presentation 21 corresponding to the case ii) is chosen.

- *Step 4*: It verifies that the hypothesis of Proposition 1.2 is valid for all $\theta \in \Omega_q$.
- *Step 5*: It gives y^2 for the Wronskian which is not equal to zero.
- *Step 6-7*: The exhaustive summary is $\{\theta_1\}$. Its analysis leads to

$$\{\bar{\theta}_1 - \theta_1, \dot{\bar{\theta}}_4, \dot{\bar{\theta}}_3, \dot{\bar{\theta}}_4\}. \quad (23)$$

and the model is not algebraically identifiable.

Finally the characteristic presentation iii) corresponds to a degenerate and unrealistic solution. The computation time of all these steps on a Pentium 4 with 2.2MHz is 1s.

5.2 A real pharmacokinetic model

Now a real pharmacokinetic model [5] is considered. It is an uncontrolled model and it was solved by pen and paper in [11]:

$$\begin{cases} \dot{x}_1 &= \alpha_1(x_2 - x_1) - \frac{V_m x_1}{k_c + x_1} \\ \dot{x}_2 &= \alpha_2(x_1 - x_2) \\ y &= x_1 \end{cases} \quad (24)$$

The unknown vector parameter is $\theta = \{\alpha_1, \alpha_2, k_c, V_m\}$.

Here are the different steps of **Algo**:

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

$$\begin{cases} \dot{x}_1(k_c + x_1) &= \alpha_1(x_2 - x_1)(k_c + x_1) - (V_m x_1) \\ \dot{x}_2 &= \alpha_2(x_1 - x_2) \\ y &= x_1 \\ k_c + x_1 &\neq 0 \end{cases} \quad (25)$$

- *Step 2*: The field of constants \mathbb{R} is chosen and the standard ranking is implicitly introduced.
- *Step 3*: **Algo** returns two cases:

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

$$\begin{cases} x_1 - y, \\ -\alpha_1 k_c x_2 - \alpha_1 x_2 y + y k_c + \alpha_1 y + V_m y, \\ 2k_c \ddot{y} y + k_c^2 \ddot{y} + (\alpha_1 + \alpha_2) \dot{y} y^2 + 2k_c (\alpha_1 + \alpha_2) \dot{y} y + ((\alpha_1 + \alpha_2) k_c + V_m) k_c \dot{y} \\ + \alpha_2 V_m y^2 + \alpha_2 V_m k_c y - \dot{y} y^2, \\ \dot{\alpha}_1, \dot{\alpha}_2, \dot{V}_m, \dot{k}_c. \end{cases} \quad (26)$$

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

$$\{\dot{x}_2 - \alpha_2 y + \alpha_2 x_2, x_1 - y, \dot{y}(k_c + y) + V_m y, \alpha_1, \dot{\alpha}_2, \dot{V}_m, \dot{k}_c\}. \quad (27)$$

The characteristic presentation (26) corresponding to the case i) is chosen.

- *Step 4:* The hypothesis of Proposition 1.2 is not valid if $V_m k_c = 0$. Indeed, with notations of Appendix C, 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 $\mathbb{R}[\theta, y, \dot{y}]$. 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 5:* It verifies that the Wronskian of

$$\{\dot{y}y, \ddot{y}, \dot{y}y^2, \dot{y}y, \dot{y}, y^2, y\} \quad (28)$$

is not in the differential ideal generated by (25).

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

$$\{k_c \alpha_2 V_m, k_c^2, k_c, k_c(\alpha_1 + \alpha_2), \alpha_2 V_m, \alpha_1 + \alpha_2, -k_c(k_c \alpha_2 + k_c \alpha_1 + V_m)\} \quad (29)$$

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

$$\{V_m - \bar{V}_m, k_c - \bar{k}_c, \alpha_1 - \bar{\alpha}_1, \alpha_2 - \bar{\alpha}_2\} \quad (30)$$

which proves that the model is rationally identifiable.

Now the characteristic presentation 27 corresponding to the case ii) is chosen.

- *Step 4:* The hypothesis of Proposition 1.2 is also not valid if $V_m k_c = 0$.

- *Step 5:* It verifies that the Wronskian of $\{\dot{y}, y\}$ is not in the differential ideal generated by (25).

- *Step 6-7:* The exhaustive summary is $\{V_m, k_c\}$ and its analysis leads to

$$\{\bar{V}_m - V_m, \bar{k}_c - k_c, \dot{\alpha}_1, \dot{\alpha}_2\}. \quad (31)$$

The model is not algebraically identifiable.

The computation time of all these steps (except step 5) on a Pentium 4 with 2.2MHz is 1.1s.

5.3 Comparison

The following example discussed in [20] and [1] is considered in order to compare the efficiency of **Algo** with another similar algorithm proposed in [1]. The model equations are:

$$\begin{cases} \dot{x}_1 &= -(k_{01} + k_{21})x_1 + k_{12}x_2 + k_{13}x_1x_3 \\ \dot{x}_2 &= k_{21}x_1 - (k_{02} + k_{12} + k_{32} + k_{42})x_2 - k_{23}x_3x_2 + k_{24}x_4 \\ \dot{x}_3 &= k_{32}x_2 - [k_{03} + k_{13}x_1 + k_{23}x_2 - k_{43}x_4]x_3 + k_{34}x_4 + u \\ \dot{x}_4 &= k_{42}x_2 + k_{43}x_3x_4 - (k_{24} + k_{34})x_4 \\ y_1 &= x_1 \\ y_2 &= x_2 \end{cases} \quad (32)$$

The unknown parameters are:

$$\theta = \{k_{01}, k_{21}, k_{12}, k_{13}, k_{02}, k_{32}, k_{42}, k_{23}, k_{24}, k_{03}, k_{43}, k_{34}\}.$$

Algo returns the characteristic presentation corresponding to the general case and an exhaustive summary of 39 equations. The analysis of this summary is purely differential and algebraic. The set $\mathbb{R}(\theta)$ is

chosen as field of constants in [1] as in **Algo** in order to compute the characteristic set and presentation. In [1] the existence of a non degenerate solution is assumed (which corresponds to the non-running of step 5 of **Algo**).

Algo leads to rational identifiability of the model and in [1] a similar result is obtained.

But in [1] a numerical random point $\theta = \{4, 6, 7, 3, 4, 6, 1, 13, 8, 12, 18, 4\}$ is chosen for constructing and analyzing the exhaustive summary, and the Groebner basis is calculated by using the Buchberger algorithm ([4]).

Algo has been implemented on a Pentium 3 with 1Mhz and on a Pentium 4 with 2.2Mhz. The computation time for this model is 25.1s (Pentium 3) and 3s (Pentium 4).

In [1] the algorithm has been implemented on a Pentium 3 with 0.55Mhz and the computation time was 509.48s.

The discrimination between computation times on Pentium 3 is specially due to the analysis of the exhaustive summary which is more efficient with **Algo** (see step7).

6 Conclusion

In this paper, we have shown how to analyze algorithmically the algebraic and rational identifiability of nonlinear controlled or uncontrolled dynamical models from an approach based on differential algebra.

The input-output approach does not make use of initial conditions but can be applied also to systems given in implicit form systems. The recent notion of characteristic presentation of a differential polynomial model is used. It summarizes all the information contained in the differential ideal into a finite number of polynomials and it supplies an effective way for testing the equality of some differential ideals. In order to apply this notion we have proved some interesting and necessary theoretical results. Characteristic presentations of input-output and exhaustive summary ideals allow the elaboration of **Algo** such that all the steps of the identifiability analysis are computed by software. Moreover, **Algo** may do an exhaustive analysis of particular cases and has been compared to an another algorithm.

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

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Appendix A. Commutative algebra

Let K be a field, X be an ordered alphabet and $K[X]$ be a polynomial ring. Let p be a non constant polynomial in $K[X]$. The *leader* of p is the greatest indeterminate x of X which occurs in p . We denote by d the highest power of this variable in p . The *separant* s_p of p is the partial derivative of p with respect to the leader x while the *initial* i_p is the coefficient of x^d .

Given $A \subset K[X] \setminus K$, H_A denotes the set of initials and separants of its elements. A is said to be *triangular* if its elements have distinct leaders. A polynomial p is said to be *strongly normalized* with respect to (w.r.t) A if no leader of A occurs in the initial of p . The set A is said to be *strongly normalized* if every p in A is strongly normalized w.r.t $A \setminus \{p\}$.

Let p and q be two polynomials over $k[X] \setminus K$. p is *lower than* q or that p is *lower ranked than* q :

- if the leader of p is lower than the leader of q ,
- or if, p and q have the same leader u and the degree d of u in p is lower than the degree of u in q .

The notation $p \simeq q$ means that two polynomials have the same leader and the same degree in this variable.

If R is a unique factorization domain and $p \in R[X]$ then p can be rewritten as $p = a_0 t_0 + \dots + a_k t_k$, where each t_i is a power product of elements of X and each a_i is in R . The *content* of p over R is the highest common factor of its coefficients, i.e. $cont(p) = gcd(a_0, \dots, a_k)$. The primitive part of p over R is the polynomial $pp(p) = \frac{p}{cont(p)}$. A polynomial is said to be *primitive* if it is equal to its primitive part.

Let \mathcal{I} be an ideal over $K[X]$. If $S = \{s_1, \dots, s_t\}$ is a finite family of elements of $K[X]$ then the *saturation* of \mathcal{I} by S , noted $\mathcal{I}:S^\infty$, is the ideal:

$$\mathcal{I}:S^\infty = \{p \in K[X] \mid \exists (n_1, \dots, n_t) \in \mathbf{N}^t, s_1^{n_1} \dots s_t^{n_t} p \in \mathcal{I}\}. \quad (33)$$

Appendix B. Differential algebra: reduction

With the notations of the introduction, a *ranking* R is a well-ordering over the indeterminates and their derivatives with the following properties for every $u, v \in \Theta V$ and $\delta \in \Delta$:

1. $u \prec \delta u$,
2. $u \prec v \Rightarrow \delta u \prec \delta v$.

Rankings such as $\{u \prec v \Rightarrow \delta u \prec \phi v\}$ (for every $\delta \in \Delta$ and $\phi \in \Delta$, and every $v, u \in \Theta V$) are said to be *elimination* rankings and are written $[u] \prec [v]$.

With a given ranking, the alphabet ΘV is ordered and the leader, the separant, the initial... well defined.

Let v be the leader of p and d be the degree of p in this variable. A differential polynomial q is said to be *partially reduced* w.r.t p if no proper derivative of v occurs in q . It is said to be *reduced* w.r.t p if it is partially reduced w.r.t p and $\deg(q, v) \leq d$.

Let a set $A \subset K\{V\} \setminus K$. A is said *differentially triangular* if it is a triangular set and if its elements are pairwise partially reduced. Moreover, A is said to be *autoreduced* if its elements are pairwise reduced. Let us notice that every autoreduced set is differentially triangular.

Let $A = A_1, A_2, \dots, A_r$ et $B = B_1, B_2, \dots, B_s$ be two autoreduced sets, A is *lower than* B if one of the two following properties is true:

1. $A_j \simeq B_j$ et $A_i < B_i$, $1 \leq j < i \leq \min(r, s)$,
2. $A_j \simeq B_j$ et $r > s$, $1 \leq j \leq s$.

Appendix C. Differential algebra: characteristic presentation

A *differential ideal* of $K\{V\}$ is an ideal of $K\{V\}$ which is stable under derivation. Let \mathcal{J} be a differential ideal of $K\{V\}$ and R be a ranking.

A set $\mathcal{D} \subset \mathcal{J}$ is a *characteristic set* if \mathcal{D} is autoreduced and \mathcal{J} contains no nonzero polynomial reduced w.r.t \mathcal{D} .

Given a set $\mathcal{C} \subset \mathcal{J}$, we now introduce the following notations:

- L denotes the set of the leaders of the elements of \mathcal{C} ,
- N denotes the other derivatives occurring in \mathcal{C} ,
- $[\mathcal{C}]$ is the differential ideal generated by the elements of \mathcal{C} .

A set $\mathcal{C} \subset \mathcal{J}$ is a *characteristic presentation* of $[\mathcal{C}] : H_{\mathcal{C}}^{\infty}$ (see (33)) if and only if \mathcal{C} is a characteristic set of $[\mathcal{C}] : H_{\mathcal{C}}^{\infty}$ and \mathcal{C} is a strongly normalized autoreduced set of $K[L, N]$ such that the elements of \mathcal{C} are primitive over $K[N]$ (see [3]).

This notion supplies an effective way for testing the equality of two regular ideals: such ideals are equal if and only if, once endowed with the same ranking, their characteristic presentation contains the same polynomials (the characteristic presentations are said equal).

Appendix D. Symbolic Computation: Rosenfeld-Groebner algorithm [2]

Differential algebra gives some algorithmic methods to solve questions appearing in the analysis of partial or ordinary differential equations: how can some variables be eliminated? do some solutions exist?

Given a differential system Σ written as polynomial equations ($p_k = 0$, $k = 1, \dots, N$) in the differential indeterminates V , these differential polynomials generate a differential ideal (denoted by \mathcal{I}), i.e. a set closed under sum, product and derivation. Moreover, the radical (denoted by $\sqrt{\mathcal{I}}$) of \mathcal{I} is the ideal of all the differential polynomials, one power of which lies in \mathcal{I} . The existence of system Σ solutions is given by the following theorem:

Theorem 6.1 [2] *Let Σ be a system of differential polynomials over $K\{V\}$ where K is a differential field of characteristic zero and \mathcal{I} the differential ideal generated by Σ . A differential polynomial q vanishes on every solution of Σ , in every differential field extension of K , if and only if q lies in $\sqrt{\mathcal{I}}$.*

This gives an easy way to test if a differential polynomial q lies in a differential ideal. Indeed, if $\sqrt{\mathcal{I}}$ admits a characteristic presentation denoted by \mathcal{C} , $q \in \sqrt{\mathcal{I}}$ if and only if q is reduced w.r.t \mathcal{C} .

Moreover, an algorithm implemented within a package in symbolic computation permits the treatment of this question [2]. Technically, from a finite set of differential polynomials and a given ranking, Rosenfeld-Groebner algorithm computes a list (understand "intersection") of characteristic presentations $\mathcal{C}_1, \dots, \mathcal{C}_j$ of regular differential ideals $\mathcal{I}_1, \dots, \mathcal{I}_j$ ($\mathcal{I}_k = [\mathcal{C}_k]:H_{\mathcal{C}_k}^\infty, k = 1, \dots, j$) so that

$$\sqrt{\mathcal{I}} = \mathcal{I}_1 \cap \mathcal{I}_2 \cap \dots \cap \mathcal{I}_j. \quad (34)$$

Informally, the different ideals \mathcal{I}_k correspond to different classes of solutions. In particular, the algorithm separates the solutions of Σ which do not depend on the same number of arbitrary constants.