

Article

An Algebraic Approach to Identifiability

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Abstract: This paper addresses the problem of identifiability of nonlinear polynomial state-space systems. Such systems have already been studied via the input-output equations, a description that, in general, requires differential algebra. The authors use a different algebraic approach, which is based on distinguishability and observability. Employing techniques from algebraic geometry such as polynomial ideals and Gröbner bases, local as well as global results are derived. The methods are illustrated on some example systems.

Keywords: identification; identifiability; observability; polynomial dynamical systems; algebraic methods; Lie derivative



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1. Introduction

Dynamical systems are usually described by a set of differential or differential-algebraic equations. These mathematical models may originate from physical laws and the known structure of that system. Such models include physical parameters, which are either known to high precision such as natural constants or depend on the geometry. Typically, some further parameter values can be measured directly, such as masses or resistance values. Contrary to that, some models are described by a parametric ansatz to reflect the system dynamics by rather simple but sufficiently accurate equations. A typical example of the latter parameters are friction coefficients, which are determined from experiments of the dynamical system. The estimation of these unknown parameters from measured data is called *parameter, process or system identification* [1,2].

The problem of parameter identification is that it asks for the determination of the model parameters from the systems input-output behaviour in order to get concrete values for a particular system instance. There is a wide range of literature on identification methods, e.g., see [1–7] and references cited there. The identified parameter values may be used to implement a precise simulation model to predict the model's behaviour or to design open-loop and closed-loop control devices.

Should it be necessary to determine unknown parameters experimentally, then the question immediately arises as to what extent this is possible at all. This problem leads directly to the question of the identifiability of the concerned parameters [8,9]. Roughly speaking, a model is identifiable, if the unknown parameters can uniquely be determined experimentally. This problem has two aspects, namely the question whether the measured data contains enough information and the question whether the systems structure allows the experimental determination [1,9]. The first question concerns the excitation of the model with appropriate test signals [10]. This paper addresses the second question with the focus on nonlinear systems.

The topic has developed the branches of structural and practical identifiability [11]. Structural identifiability asks for the feasibility to compute the parameters from the input-output behaviour of the mathematical model without noise or uncertainties. This is often not useful if the identification problem is ill-conditioned. Practical identifiability

also addresses the quality of the measurements and its implication on the quality of the identified parameters.

Identification and identifiability are related to several other problems in control theory. The most obvious connection is to observer design and observability, which concerns the estimation of the system's state [9,12–15]. In [16,17], the authors carry out the identification by means of adaptive control. The combination with the previous approach results in adaptive observers [18,19]. A further relation concerns the field of fault detection, i.e., the detection of changing system properties over the time, see [14,20].

In the literature, identifiability is defined in different ways depending on the context [1,9,20]. As this article deals with structural algebraic methods, the definitions that seem most common are used herein. Note that what is called locally identifiability herein is sometimes referred to as structural identifiability, see [21]. The algebraic identifiability approaches mostly examine the differential input-output relations by eliminating the state variables over a differential ring [22–25]. This leaves one with a set of equations of the known input and output trajectories and the parameters. Identifiability then asks for the solvability for the parameters. This elimination can be done over the differential polynomial ring using the well-known Ritt algorithm [26].

This article considers a method that does not rely on a differential ring and can determine the identifiability using computations in the ordinary polynomial ring [27–29] alone. The computation in this simpler domain comes at the cost of more variables that are required to formulate the problem. This approach is based on an observability criterion [30–32] and is extended to an identifiability criterion for polynomial systems. [A note to the difference and extension from the observability criterion as suggested by reviewer 1 and reviewer 3 point 1.] In contrast to the observability test, the distinguishability is concerned differently for state variables and parameters. This will be translated into the algebraic context.

As suggested by the academic editor, a note to the polynomial system class is inserted. Many chemical reactions or biological systems are described by such polynomial differential equations. Even for linear electrical networks, the physical parameters, such as resistance and capacitance, usually appear in products, yielding polynomials of the parameters in the differential equations. Some other systems can be recast into a polynomial form using an embedding into a higher-dimensional space. Those embeddings can be handled as well.

The paper structures as follows: In Section 2, we provide the required mathematical preliminaries. The main results are stated in Section 3. Our approach is illustrated on several example systems in Section 4. Finally, the results obtained will be discussed in Section 5.

2. Preliminaries

Let $\Theta \subseteq \mathbb{R}^s$ be a semi-algebraic set of parameter-tuples, i.e., a subset of \mathbb{R}^s described by a boolean combination of polynomial equations and inequalities. For each parameter-tuple $p \in \Theta$, consider a real-analytic manifold $\mathcal{M}_p \subseteq \mathbb{R}^n$ and the dynamic system

$$\dot{x} = f_0(x; p) + \sum_{k=1}^m f_k(x; p)u_k \quad (1a)$$

$$y_k = h_k(x; p), \quad k = 1, \dots, l \quad (1b)$$

with vector fields $f_0, f_k : \mathcal{M}_p \rightarrow T\mathcal{M}_p$ and real-analytic scalar fields $h_k : \mathcal{M}_p \rightarrow \mathbb{R}$. Herein, x , u , and y denote the system state, input, and output, respectively. Furthermore, the parametric manifold \mathcal{M}_p is the real variety of a polynomial ideal $\langle c_1, \dots, c_j \rangle \subset \mathbb{R}[x, p]$, and the components of f_0, f_k as well as h_k are polynomials in $\mathbb{R}[x, p]$.

In the context of parameter identification, the system state is usually extended to contain the parameters too, which obey the simple differential equation:

$$\dot{p} = 0. \quad (1c)$$

One has to ensure that the initial value $p(0) \in \Theta$ is chosen such that \mathcal{M}_p is a manifold. Note that \mathcal{M}_p may be singular for some $p \notin \Theta$. This allows to consider identifiability as a special case of observability, where a subset p of the extended system state $(x; p)$ is to be determined from the input and output trajectories.

For nonlinear systems, observability is defined using the concept of the indistinguishability of states: Two system states $x, \bar{x} \in \mathcal{M}_p$ are said to be *distinguishable* if and only if there exists an interval $[0, T[$ with $T > 0$ and a piecewise constant input $u : [0, T[\rightarrow \mathbb{R}^m$ such that the output trajectories $h(x(t); p)$ of Equation (1) corresponding to initial conditions $x(0) = x$ and $x(0) = \bar{x}$, respectively, differ in that interval. Contrarily, if the output trajectories are identical, the states are called *indistinguishable*.

This can also be applied to the extended state $(x; p)$ or formulated for distinguishability in the parameters only, if the initial condition $x(0)$ is known, as opposed to the observability case, where the parameters are supposed to be known.

2.1. Differential Equations and Their Flow

Consider an autonomous system first, i.e., the vector field in Equation (1a) does not depend on an input u . The *flow* $\varphi_t : \mathcal{M}_p \rightarrow \mathcal{M}_p$ of Equation (1a) is the general solution $x(t) = \varphi_t(x_0)$ of Equation (1a) at time t with initial value $x(0) = x_0$. Since the vector field in Equation (1a) is a polynomial in x and, therefore, is locally Lipschitz continuous, the Picard–Lindelöf Theorem ensures that the flow $\varphi_t(x_0)$ is locally analytic in t . The same holds for the output trajectories $y_k(t) = h_k(\varphi_t(x_0))$. This allows to expand the output trajectories in terms of their *Lie series*

$$y_k(t) = \sum_{i=0}^{\infty} \frac{t^i}{i!} L_{f_0}^i h_k(x(0); p), \quad k = 1, \dots, l,$$

where $L_f^i h$ denotes the i -th *Lie derivative* of h along the vector field f , defined by

$$\begin{aligned} L_f h(x) &= \frac{dh}{dx}(x) f(x) \\ L_f^0 h(x) &= h(x) \\ L_f^{i+1} h(x) &= L_f L_f^i h(x), \end{aligned}$$

see [33]. For notational convenience, we use the same notation for a vector of scalar fields. In this case, the Lie derivative of a vector of scalar fields yields a vector of scalar fields again, where the (usual) Lie derivative is applied to each vectorial component [34]. This is not to be confused with the Lie derivative of a vector field defined in a different way.

If the system is forced by piecewise constant inputs

$$u_k(t) = u_k^i \in \mathbb{R} \text{ for } T_i \leq t < T_{i+1} = T_i + \tau_{i+1}$$

with $T_0 = 0, \tau_i > 0, k = 1, \dots, m$, one may write

$$f^i = f_0 + \sum_{k=1}^m f_k u_k^i$$

and gets

$$x(T_N) = \varphi_{\tau_N}^{f^N} \circ \dots \circ \varphi_{\tau_1}^{f^1}(x(0))$$

for the solution of Equation (1a) at time T_N , which is the composition of the flows. Here, there are different flows depending on the current vector field.

2.2. Ideals and Varieties

The succeeding sections will make use of polynomial ideals and their corresponding varieties. Therefore, the required concepts used herein are briefly introduced as well.

Consider the commutative multivariate polynomial ring $\mathbb{R}[x_1, \dots, x_n] = \mathbb{R}[x]$ in the variables x_1, \dots, x_n . An ideal $I \subseteq \mathbb{R}[x]$ is a special subset of this ring satisfying the conditions

1. $0 \in I$
2. $a, b \in I \implies a + b \in I$
3. $a \in I, c \in \mathbb{R}[x] \implies ca \in I$.

Thus, an ideals contains an infinite number of polynomials, let alone the trivial ideal $\{0\}$. Nonetheless, Hilbert’s basis theorem asserts that these ideals can be represented using a finite polynomial set $G = \{g_1, \dots, g_s\} \subset \mathbb{R}[x]$, a so-called basis, by

$$I = \langle g_1, \dots, g_s \rangle = \{a_1g_1 + \dots + a_sg_s \mid a_1, \dots, a_s \in \mathbb{R}[x]\}.$$

There are different bases that represent the same ideal, possibly with a different number of generators. Ideals can be compared by computing a so-called standard basis or *Gröbner basis*. A reduced Gröbner basis is unique for a given monomial ordering, and there is an algorithm to compute them. On the other hand, one can easily verify whether a polynomial is contained in an ideal given a Gröbner basis of that ideal. This allows deciding subset relations of ideals (and thus also their equality).

The common real zero set $V = \mathbf{var}^{\mathbb{R}}(I) \subseteq \mathbb{R}^n$ of all polynomials in an ideal $I \subseteq \mathbb{R}[x]$ is called the *real variety* of that ideal. This mapping from ideals to varieties is not bijective. Consider, for example, the ideals $\langle x \rangle, \langle x^2 \rangle \subseteq \mathbb{R}[x]$ over the univariate ring, which are different, but whose real varieties $\{0\} \subseteq \mathbb{R}$ coincide. Given a real variety $V \subseteq \mathbb{R}^n$, there is, however, an ideal $\text{Id}(V) \subseteq \mathbb{R}[x]$ containing all polynomials that vanish on V . Such an ideal is called *real*, and there is a one-to-one correspondence between real ideals and real varieties. This real ideal is the superset of all ideals whose polynomials evaluate to zero on the real variety and is called the *real radical* of that ideals. The real radical $\mathbf{rad}^{\mathbb{R}}(I)$ of an ideal I can also be computed algebraically [29, p. 85]. One can also consider the set of polynomials in $\mathbb{R}[x]$ that vanish on a set $W \subseteq \mathbb{R}^n$, which is not a real variety. These polynomials will then have additional zeros

$$W \subseteq \mathbf{var}^{\mathbb{R}}(\text{Id}(W)) = \overline{W} \subseteq \mathbb{R}^n.$$

This variety \overline{W} is called the *Zariski closure* of W , the smallest variety containing W .

Like the real radical, there is a correspondence of geometric set operations on the varieties and operations on the ideals, which make it possible to handle these operations algebraically.

The intersection $V \cap W$ of real varieties corresponds to the *sum* $I + J$ of the ideals I and J :

$$\mathbf{var}^{\mathbb{R}}(I + J) = \mathbf{var}^{\mathbb{R}}(I) \cap \mathbf{var}^{\mathbb{R}}(J).$$

The sum is defined as the set of all polynomials contained in I or J and is also an ideal. For the union of varieties, one has

$$\mathbf{var}^{\mathbb{R}}(I \cap J) = \mathbf{var}^{\mathbb{R}}(I) \cup \mathbf{var}^{\mathbb{R}}(J),$$

where

$$I \cap J = \{g \mid g \in I \wedge g \in J\}$$

is the *intersection* of the ideals.

The difference set $V \setminus W$ of two varieties V and W is, in general, not a variety anymore. As an example, consider in \mathbb{R}^1 the varieties $V = \mathbb{R}$ and $W = \{0\}$ with corresponding real ideals $\langle 0 \rangle$ and $\langle x \rangle$, respectively. There is no ideal with real variety $V \setminus W$. However, there is an algebraic counterpart to the Zariski closure of the difference set:

$$\mathbf{var}^{\mathbb{R}}(I : J^\infty) = \overline{\mathbf{var}^{\mathbb{R}}(I) \setminus \mathbf{var}^{\mathbb{R}}(J)}$$

with the saturation ideal

$$I : J^\infty = \{g \mid gh^N \in I \text{ for some } N \text{ and all } h \in J\}.$$

A real variety might allow to be written as a union of varieties. Such a decomposition

$$V = V_1 \cup \dots \cup V_s$$

is said to be *irreducible* if the varieties cannot be decomposed further and are not subsets of each other. To this decomposition as a union corresponds a decomposition of the ideal, written as an intersection of *prime* ideals.

2.3. Indistinguishability of States

First consider an autonomous system

$$\dot{x} = f(x), y = h(x) \tag{2}$$

with $f : \mathcal{M} \rightarrow T\mathcal{M}, h : \mathcal{M} \rightarrow \mathbb{R}^l$, where the system state and parameters are condensed in the variables $x \in \mathcal{M}$ for a moment. As previously noted, two system states $x, \bar{x} \in \mathcal{M}$ are said to be distinguishable if and only if there exists an interval $[0, T]$ such that the output trajectories $h(x(t))$ corresponding to initial conditions $x(0) = x$ and $x(0) = \bar{x}$, respectively, differ in that interval.

As the output trajectories are locally analytic, there is a one-to-one correspondence between the trajectory and the coefficients of the Lie-series. Thus, the distinguishability can be equivalently expressed in terms of the *observability map*

$$q(x) = \begin{pmatrix} h(x) \\ L_f h(x) \\ L_f^2 h(x) \\ \vdots \end{pmatrix}$$

as follows: Two states $x, \bar{x} \in \mathcal{M}_p$ are indistinguishable if and only if

$$q(x) = q(\bar{x}) \implies x = \bar{x}. \tag{3}$$

This formula, however, is to some extent unsatisfying as it contains an infinite number of equations. In [32], this problem has been handled for the case of polynomial vector fields and output maps. The key of this approach is to use two copies of Equation (2) with a vector field

$$F : \mathcal{M} \times \mathcal{M} \rightarrow T(\mathcal{M} \times \mathcal{M}) \\ F(x, \bar{x}) = f(x) \frac{\partial}{\partial x} + f(\bar{x}) \frac{\partial}{\partial \bar{x}}$$

and output map

$$H(x, \bar{x}) = h(x) - h(\bar{x}).$$

This way the components of the residuum observability map

$$Q(x, \bar{x}) = q(x) - q(\bar{x}) \tag{4}$$

are precisely the Lie derivatives $L_F^i H(x, \bar{x}), i = 0, 1, 2, \dots$. The common zero-set of Q is an algebraic variety; thus, the set of polynomials in $\mathbb{R}[x, \bar{x}]$ that vanish on that variety is finitely generated by Hilbert's basis theorem. This polynomial ideal is generated by the polynomials $H_k \in \mathbb{R}[x, \bar{x}], k = 1, \dots, l$ as well as their (higher-order) Lie derivatives along the vector field F . As L_F is a derivative operator $L_F : \mathbb{R}[x, \bar{x}] \rightarrow \mathbb{R}[x, \bar{x}]$, a generating set for the ideal generated by the components of the extended observability map Q can be computed in a finite number of steps, see [31,32,35].

A very simple yet computationally suboptimal algorithm starts with a generating set

$$G_0 = \{H_1, \dots, H_l\}$$

of the output maps and iteratively adds their (extended) Lie derivatives along F :

$$G_{k+1} = G_k \cup \{L_F^k H_1, \dots, L_F^k H_l\}.$$

The such generated ideals form an ascending chain

$$\langle G_0 \rangle \subseteq \langle G_1 \rangle \subseteq \dots \subseteq \langle G_N \rangle = \langle G_{N+1} \rangle = \dots \stackrel{\text{def}}{=} L_F^\infty \langle G_0 \rangle \tag{5}$$

that terminates after a finite number of steps by the ascending chain condition, yielding a finite generating set G_N . Now, Equation (3) can be written using a finite number of atomic formulas:

$$\bigwedge_{g \in G_N, \langle G_N \rangle = L_F^\infty \langle G_0 \rangle} g(x, \bar{x}) = 0 \implies x = \bar{x}.$$

2.4. The Nonautonomous Case

If the vector field depends on an input, two states are called indistinguishable if and only if the corresponding output trajectories are equal for all piecewise constant inputs. Using a similar notation

$$\begin{aligned} \dot{x} &= f_0(x) + \sum_{k=1}^m f_k(x) u_k \\ y &= h(x) \end{aligned}$$

with condensed state and parameters in the variables x and a piecewise constant input

$$u(t) = u^i \in \mathbb{R}^m \text{ for } T_i \leq t < T_{i+1} = T_i + \tau_i$$

with $T_0 = 0$, $\tau_i > 0$, and corresponding vector fields

$$f^i = f_0 + \sum_{k=1}^m f_k u_k^i,$$

one can expand the output trajectory with initial value x_0 locally for sufficiently small τ_i :

$$y(T_N) = \sum_{k \in \mathbb{Z}_{\geq 0}^N} \frac{\tau_1^{k_1} \dots \tau_N^{k_N}}{k!} L_{f^N}^{k_N} \dots L_{f^1}^{k_1} h(x_0),$$

see [36]. As indistinguishable initial conditions yield the same output trajectory for any input, all coefficients in this Lie series, i.e., all mixed Lie derivatives must be equal. Thus, the polynomials that vanish on indistinguishable pairs are contained in the ideal

$$I_0 = \langle H_1, \dots, H_l \rangle$$

closed under all derivative operators L_F with F of the form

$$F(x, \bar{x}) = f^i(x) \frac{\partial}{\partial x} + f^i(\bar{x}) \frac{\partial}{\partial \bar{x}}$$

parameterized by an input $u^i \in \mathbb{R}^m$. Since the Lie derivative is a linear operator, it suffices to close the ideal under the finitely many operators L_{F_k} with

$$F_k(x, \bar{x}) = f_k(x) \frac{\partial}{\partial x} + f_k(\bar{x}) \frac{\partial}{\partial \bar{x}}, \quad k = 0, 1, \dots, m.$$

Again, this can be done by computing a chain

$$I_0 \subseteq I_1 \subseteq \dots \subseteq I_N = I_{N+1} = \dots$$

of ideals, where

$$I_{k+1} = I_k + \langle L_{F_0}g, L_{F_1}g, \dots, L_{F_m}g \mid g \in I_k \rangle.$$

We will write the stabilized ideal as

$$L_{F_0, F_1, \dots, F_m} \langle H_1, \dots, H_l \rangle.$$

3. Observability and Identifiability

In this section, observability and identifiability of systems of Equation (1) is discussed using the notation introduced in Section 2. Furthermore, instead of writing $L_{F_0, F_1, \dots, F_m} I$ for the stabilized Lie derivative of an ideal I with respect to all vector fields F_k , we write \mathcal{F} for the linear span of the latter vector fields and $L_{\mathcal{F}}$ for the corresponding operator acting on ideals. This clearly includes the autonomous case, where the space \mathcal{F} is one-dimensional, i.e., spanned by the single vector field F_0 .

3.1. Global Identifiability and Observability

We discuss the most general case with an extended state $z = (x, \bar{x}; p, \bar{p})$ containing two copies of the state and parameter tuple first. The space $\mathcal{Z} = \mathcal{M}_p \times \mathcal{M}_{\bar{p}} \times \Theta^2$ of the extended states is a semi-algebraic set; thus, its Zariski closure is the real variety of an ideal \mathfrak{Z} . This ideal is generated by all equations governing the manifolds \mathcal{M}_p and $\mathcal{M}_{\bar{p}}$ and possibly the parameter space Θ^2 if the parameters are not independent of each other. Within the set of extended states, one may identify equal extended states, e.g., the subset

$$\mathcal{J} = \left\{ z = (x, \bar{x}; p, \bar{p}) \in \mathcal{Z} = \mathcal{M}_p \times \mathcal{M}_{\bar{p}} \times \Theta^2 \mid x = \bar{x} \wedge p = \bar{p} \right\} \tag{6}$$

of equal states and parameters for each system copy. The main question is if that set of equal extended states matches the set $\mathcal{I} \subseteq \mathcal{Z}$ of indistinguishable states. As the equal states are obviously indistinguishable, one has $\mathcal{I} \supseteq \mathcal{J}$, and it suffices to test if the reverse inclusion holds.

Assume for a moment that \mathcal{J} in Equation (6) is a real variety, i.e., the parameter set Θ is an algebraic yet not semi-algebraic set. This means that the space \mathcal{Z} of extended states is the real variety of a real ideal \mathfrak{Z} and that the varieties in Equation (6) correspond to a real ideal

$$\mathfrak{J} = \mathfrak{Z} + \langle x_1 - \bar{x}_1, \dots, x_n - \bar{x}_n, p_1 - \bar{p}_1, \dots, p_s - \bar{p}_s \rangle \subset \mathbb{R}[x, \bar{x}, p, \bar{p}].$$

Furthermore the set \mathcal{I} of indistinguishable states equals the real variety of the stabilized ideal $L_{\mathcal{F}}^{\infty} \langle H_1, \dots, H_l \rangle$ of the extended output maps, where \mathcal{F} is the linear span of the extended vector fields

$$F_k(x, \bar{x}; p, \bar{p}) = f_k(x; p) \frac{\partial}{\partial x} + f_k(\bar{x}; \bar{p}) \frac{\partial}{\partial \bar{x}}. \tag{7}$$

The equality of the indistinguishable and equal states can be tested by comparing the corresponding real ideals

$$\mathfrak{J} = \mathfrak{Z} + \mathbf{rad}^{\mathbb{R}}(L_{\mathcal{F}}^{\infty} \langle H_1, \dots, H_l \rangle) \tag{8}$$

and \mathfrak{J} . Note that the ideal sum with \mathfrak{Z} is necessary to restrict the states to the manifold they are contained in.

In many cases, the parameter space is not algebraic because of physical restrictions, e.g., a mass is usually restricted to positive values. In this case, \mathfrak{Z} is taken to be the real ideal corresponding to the Zariski closure of \mathcal{Z} . Then, however, the variety $\mathbf{var}^{\mathbb{R}}(\mathfrak{J})$ may contain irreducible components that do not respect these restrictions, e.g., lie in a plane where the mass vanishes. In such cases, the comparison of the ideals \mathfrak{J} and \mathfrak{J} is not sufficient to test global identifiability.

Therefore, we compute the decomposition of \mathfrak{J} into its minimal associated primes

$$\mathfrak{J} = \mathfrak{J}_1 \cap \dots \cap \mathfrak{J}_k$$

and check if the corresponding irreducible varieties lie in the extended state and parameter space:

$$\exists x, \bar{x}, p, \bar{p} : (x, \bar{x}, p, \bar{p}) \in \mathcal{Z} \cap \mathbf{var}^{\mathbb{R}}(\mathcal{J}_i), \quad i = 1, \dots, k. \tag{9}$$

The set can be described by a boolean combination of equations and inequalities. Note that the equations are the collections of the form $g(x, \bar{x}, p, \bar{p}) = 0$ with all polynomials g in the generators of $\mathcal{J}_i \supseteq \mathfrak{J}$. The quantified Equation (9) can always be transformed into a quantifier-free formula [37,38]. If the quantifier-free equivalent to Equation (9) is FALSE for some \mathcal{J}_i , then the corresponding real variety $\mathbf{var}^{\mathbb{R}}(\mathcal{J}_i)$ is disjoint from the admissible extended state and parameter space \mathcal{Z} , and we set $\hat{\mathcal{J}}_i = \langle 1 \rangle$. Otherwise, i.e., the quantifier-free equivalent is TRUE, there are indistinguishable tuples in \mathcal{Z} , and we set $\hat{\mathcal{J}}_i = \mathcal{J}_i$. We collect all these components and write

$$\hat{\mathcal{J}} = \bigcap_{i=1}^k \hat{\mathcal{J}}_i.$$

The real variety $\mathbf{var}^{\mathbb{R}}(\hat{\mathcal{J}})$ is then the Zariski closure of the indistinguishable states $\mathcal{I} \subseteq \mathcal{Z}$.

Using this notation, we are able to express the global identifiability as follows: The system in Equation (1) is globally identifiable and globally observable if and only if $\hat{\mathcal{J}} = \mathfrak{J}$. Note that if the system is globally identifiable and observable, this holds for any initial condition of the system state x .

With small variations on the ring and the ideals, other properties can be tested as well:

3.2. Global Identifiability with Known Initial Conditions

The question arises if the parameters can be distinguished from the output trajectories if the system is known to be in a definite state, which usually simplifies the identification problem. There is only a small modification necessary compared to the general case, namely that the indistinguishable states are intersected with the plane $x = \bar{x}$. This can be accomplished by substituting Equation (8) with

$$\mathfrak{J} = \mathfrak{J} + \mathbf{rad}^{\mathbb{R}}(\mathcal{L}_{\mathcal{F}}^{\infty}\langle H_1, \dots, H_l \rangle) + \langle x_1 - \bar{x}_1, \dots, x_n - \bar{x}_n \rangle.$$

Note that one cannot easily get rid of the copied state variables \bar{x} until this point as these are required to distinguish the system copies when taking the Lie derivatives with respect to Equation (7), where the different parameters matter. The remaining test can be applied as in the general case before.

3.3. Global Identifiability

When one wants to decide if a system is identifiable without bothering if the initial condition can be restored from the output trajectory, the statement at the end of Section 3.1 is too restrictive. However, instead of comparing the sets \mathcal{I} and \mathcal{J} that contain the full extended state, one may compare these sets in their projections on the parameter plane

$$\{(x, \bar{x}, p, \bar{p}) \in \mathcal{Z} \mid x = \bar{x} = 0\}.$$

This corresponds algebraically to the comparison of the *elimination ideals*

$$\hat{\mathcal{J}} \cap \mathbb{R}[p, \bar{p}], \quad \mathfrak{J} \cap \mathbb{R}[p, \bar{p}].$$

The system is globally identifiable if and only if these ideals are equal, regardless of the initial condition.

3.4. Global Identifiability of a Particular Parameter

The statement that a system is not identifiable is not always satisfying. In some cases, only a subset of the parameters can be identified. Thus, it makes sense to test the identifiability for each parameter p_i . This can be accomplished by computing further elimi-

nations as in the preceding section, namely by comparing the elimination ideals $\hat{\mathfrak{J}} \cap \mathbb{R}[p_i, \bar{p}_i]$ and $\mathfrak{J} \cap \mathbb{R}[p_i, \bar{p}_i]$.

3.5. Global Observability

For the observability test, the parameters are assumed to be known. Therefore, the extended state space is restricted to $\mathcal{Z} = \mathcal{M}_p^2 \times \Theta \ni z = (x, \bar{x}, p)$. We identify equal extended states by

$$\mathcal{J} = \{z = (x, \bar{x}; p) \in \mathcal{Z} \mid x = \bar{x}\},$$

i.e., by equal ordinary state. Thus, the corresponding ideal to the Zariski closure thereof reads

$$\mathfrak{J} = \mathfrak{J} + \langle x_1 - \bar{x}_1, \dots, x_n - \bar{x}_n \rangle \subset \mathbb{R}[x, \bar{x}; p].$$

The ideal generated by the extended output maps is closed under the Lie derivatives with respect to the vector fields

$$F_k(x, \bar{x}; p) = f_k(x; p) \frac{\partial}{\partial x} + f_k(\bar{x}, p) \frac{\partial}{\partial \bar{x}}.$$

This differs only in the part in direction $\frac{\partial}{\partial \bar{x}}$, which is evaluated at the same parameter p . Using the same notation, the system is globally observable if and only if $\hat{\mathfrak{J}} = \mathfrak{J}$. This holds for all admissible parameters.

In addition, the parameter subset for the given global observability can be computed by solving the quantifier elimination problem

$$\forall x, \bar{x} : (x, \bar{x}; p) \in \mathcal{Z} \wedge \left((x, \bar{x}; p) \in \mathbf{var}^{\mathbb{R}}(\mathfrak{J}) \implies x = \bar{x} \right).$$

3.6. Locally Identifiability

For some systems, there might be initial conditions that prevent the unique identification of parameters from the corresponding output trajectories. Common examples are equilibria of autonomous systems. The method described herein allows computing such subsets when the identifiability is not given. Apart from those subsets, the map between the initial state and parameter $(x; p)$ and the output trajectory may still be injective within a neighbourhood of a point (x_0, p_0) . This means that varieties $\mathbf{var}^{\mathbb{R}}(\hat{\mathfrak{J}}) = \bar{\mathcal{I}}$ and $\bar{\mathcal{J}}$ and the Zariski closures of indistinguishable and equal extended states, respectively, are equal in an open neighbourhood of a point $z_0 = (x_0, x_0; p_0, p_0) \in \mathcal{Z}$. The equality in this neighborhood can be tested geometrically by removing all irreducible components of the indistinguishable set \mathcal{I} that are not contained in this neighborhood. On the other hand, the points z_0 , where the varieties are not equal, are easily found as they are either contained in more than one irreducible component of $\bar{\mathcal{I}}$ or such a component strictly contains $\bar{\mathcal{J}}$, i.e., has a higher dimension.

Recall that the Zariski closure of the indistinguishable extended states is given by $\mathbf{var}^{\mathbb{R}}(\hat{\mathfrak{J}})$, where

$$\hat{\mathfrak{J}} = \hat{\mathfrak{J}}_1 \cap \dots \cap \hat{\mathfrak{J}}_k \subseteq \mathfrak{J}$$

and all ideals $\hat{\mathfrak{J}}_i$ are relatively prime. If there are some $\hat{\mathfrak{J}}_i$ that are strictly contained in \mathfrak{J} , the system is at no point locally observable or identifiable. Instead, there may be a locally or globally identifiable subspace. Otherwise, one of the prime components in the minimal decomposition must equal \mathfrak{J} (because the indistinguishable states always include the equal ones). In this case, the not locally observable points z_0 are found by intersecting \mathcal{J} with the corresponding real varieties $\mathbf{var}^{\mathbb{R}}(\hat{\mathfrak{J}}_i)$ different from the one of the equal extended states. Note that the extended point z_0 includes two copies of the same original point $(x_0; p_0)$, which is just a projection of the latter.

While there were different definitions for equal and indistinguishable pairs for different global problems in the preceding sections, the same can be used to discuss local properties, as described herein. Note that for the identifiability test for all or a subset of

the parameters, as described in Sections 3.3 and 3.4, the projection has to be done for each irreducible variety independently.

4. Examples

4.1. The Van der Pol Oscillator

The Van der Pol oscillator is considered with an increasing number of parameters. In its simplest form, the equations of motion read

$$\begin{aligned} \dot{x}_1 &= x_2 \\ \dot{x}_2 &= -x_1 - \epsilon x_2 (x_1^2 - 1) \\ y &= x_1 \end{aligned}$$

where $\epsilon \in \Theta = \mathbb{R}$ is a parameter. The chain of ideals defined by Equation (5) starting with $\langle x_1 - \bar{x}_1 \rangle$ generated by the extended output map stabilizes after the fifth Lie derivative with respect to the parametric vector field. This stabilized ideal is already real and reads

$$\mathfrak{J} = \langle x_1 - \bar{x}_1, x_2 - \bar{x}_2, x_1(\epsilon - \bar{\epsilon}), x_2(\epsilon - \bar{\epsilon}) \rangle$$

and can be written as an intersection

$$\langle x_1, x_2, \bar{x}_1, \bar{x}_2 \rangle \cap \langle x_1 - \bar{x}_1, x_2 - \bar{x}_2, \epsilon - \bar{\epsilon} \rangle$$

of prime ideals. The latter of these ideals corresponds to equal states and parameters, i.e., the ideal \mathfrak{J} . The first one describes the not identifiable part, which consists of the (sole) equilibrium $(x_1, x_2) = (0, 0)$ for each system copy. Thus, the system is locally identifiable except at the equilibrium, where the output trajectory is identically zero for all parameters ϵ .

The system is modified to include two parameters and reads

$$\begin{aligned} \dot{x}_1 &= x_2 \\ \dot{x}_2 &= -x_1 - x_2 (ax_1^2 - b) \end{aligned}$$

further on, while the output map is preserved. The chain of ideals generated by Lie derivatives of the extended output map stabilizes after the seventh Lie derivative has been added. This ideal is not yet radical. However, the radical takes a similar form

$$\mathfrak{J} = \langle x_1, x_2, \bar{x}_1, \bar{x}_2 \rangle \cap \langle x_1 - \bar{x}_1, x_2 - \bar{x}_2, a - \bar{a}, b - \bar{b} \rangle$$

as for the previous system. Again, the parameters are structurally identifiable, and the equilibrium is the only exceptional point.

If an additional parameter c is included such that

$$\begin{aligned} \dot{x}_1 &= x_2 \\ \dot{x}_2 &= -cx_1 - x_2 (ax_1^2 - b), \end{aligned}$$

Lie derivatives up to order nine are required until the chain of ideals stabilizes. The radical of the stabilized Lie derivative can be written as an intersection of five irreducible components:

$$\begin{aligned} \mathfrak{J} &= \langle x_1, x_2, \bar{x}_1, \bar{x}_2 \rangle \\ &\cap \langle x_1 - \bar{x}_1, x_2 - \bar{x}_2, a - \bar{a}, b - \bar{b}, c - \bar{c} \rangle \\ &\cap \langle x_1 - \bar{x}_1, x_2 - \bar{x}_2, a, \bar{a}, x_1(c - \bar{c}) - x_2(b - \bar{b}), x_1x_2\bar{b} - x_1^2\bar{c} - x_2^2, \\ &\quad x_2(b\bar{b} - \bar{b}^2 - c + \bar{c}) - x_1\bar{c}(b - \bar{b}), bc\bar{b} - c\bar{b}^2 - b^2\bar{c} + b\bar{b}\bar{c} - c^2 + 2c\bar{c} - \bar{c}^2 \rangle \\ &\cap \langle x_1 - \bar{x}_1, x_2 - \bar{x}_2, b, \bar{b}, ax_2^2 + c, \bar{a}x_2^2 + \bar{c}, a\bar{c} - \bar{a}c \rangle \\ &\cap \langle x_1 - \bar{x}_1, x_2 - \bar{x}_2, c, \bar{c} \rangle \end{aligned}$$

The first two components are similar to the previous cases. As the ideal \mathfrak{J} occurs in the second prime component, the system is locally identifiable again, except at the equilibrium. The remaining three components describe other constellations for that local identifiability fails. As can be seen, these correspond to degenerate parameter constellations $a = 0$, $b = 0$, or $c = 0$, respectively.

4.2. The Lotka–Volterra Model

We consider the Lotka–Volterra system given by

$$\begin{aligned} \dot{x}_1 &= ax_1 - bx_1x_2 \\ \dot{x}_2 &= -cx_2 + dx_1x_2 \\ y &= x_1 \end{aligned}$$

with measurement of the prey population x_1 . The parameters $(a, b, c, d) \in \Theta = \mathbb{R}_+^4$ are all positive.

As the system is autonomous, there is a single extended vector field. Evaluating the ideal defined by Equation (8) yields an ideal with 18 prime components. We have used a more efficient method to compute the minimal associated primes of the stabilized chain directly, as evaluating the chain of ideals defined by Equation (5) using the simple algorithm was not possible in reasonable time. Thus, we do not know up to which order Lie derivatives are required to stabilize the chain.

Most of these corresponding varieties of the prime ideals lie in a plane where at least one parameter equals zero. These components can be removed since they do not lie in the parameter space. The remaining components read

$$\begin{aligned} \hat{\mathfrak{J}}_1 &= \langle x_1, \bar{x}_1 \rangle \\ \hat{\mathfrak{J}}_2 &= \langle x_1 - \bar{x}_1, x_2, \bar{x}_2, a - \bar{a} \rangle \\ \hat{\mathfrak{J}}_3 &= \langle x_1 - \bar{x}_1, bx_2 - \bar{b}\bar{x}_2, a - \bar{a}, c - \bar{c}, d - \bar{d} \rangle \\ \hat{\mathfrak{J}}_4 &= \langle x_1 - \bar{x}_1, dx_1 - c, \bar{d}\bar{x}_1 - \bar{c}, bx_2 - a, \bar{b}\bar{x}_2 - \bar{a} \rangle. \end{aligned}$$

As one can see, the ideal

$$\mathfrak{J} = \langle x_1 - \bar{x}_1, x_2 - \bar{x}_2, a - \bar{a}, b - \bar{b}, c - \bar{c}, d - \bar{d} \rangle$$

is not under these primes, which means that the system is not locally identifiable. However, the component $\hat{\mathfrak{J}}_3$ suggests that at least a subset of the parameters are locally identifiable. Indeed, eliminating the state (x_1, x_2) , the parameter b and their copies yields

$$\hat{\mathfrak{J}}_3 \cap \mathbb{R}[a, c, d; \bar{a}, \bar{c}, \bar{d}] = \mathfrak{J} \cap \mathbb{R}[a, c, d; \bar{a}, \bar{c}, \bar{d}] = \langle a - \bar{a}, c - \bar{c}, d - \bar{d} \rangle.$$

This means that the parameters a , c , and d are locally identifiable, while b is not.

The not locally observable points include the degenerate case $x_1 = 0$, where not one parameter can be identified at all due to $\hat{\mathfrak{J}}_1$. The other degenerate case $x_2 = 0$ is also special. Eliminating all variables except a and \bar{a} in $\hat{\mathfrak{J}}_2$ and $\hat{\mathfrak{J}}_3$ yields $\langle a - \bar{a} \rangle$; thus, a is identifiable

on this line. However, only $\hat{\mathcal{J}}_3$ equals $\langle c - \bar{c} \rangle$ or $\langle d - \bar{d} \rangle$ when eliminating all but these variables, respectively. This shows that parameters c and d are not local identifiable at $x_2 = 0$. Another point for that identification fails for all parameters is the nontrivial equilibrium, indicated by $\hat{\mathcal{J}}_4$. Note that one still can get the ratio of the parameters c and d ; however, these identifiable functions are beyond the scope of this article.

4.3. Van de Vusse Reaction

An interesting nonautonomous example is the isothermal Van de Vusse reaction [39–41] described by

$$\begin{aligned}\dot{x}_1 &= -k_1x_1 - k_3x_1^2 + (c - x_1)u \\ \dot{x}_2 &= k_1x_1 - k_2x_2 - x_2u,\end{aligned}$$

where the state variables x_1 and x_2 describe concentrations in the reactor. The control input u is a normalized inlet flow rate. The reaction rates k_1 , k_2 , and k_3 as well as the inlet concentration c are positive parameters. We assume a measurement $y = x_1$ of the reactant concentration.

The chain (5) of ideals stabilizes after including the sixth Lie derivative with respect to both the drift and control vector field. Writing the radical of the latter as an intersection of irreducible ideals yields 19 components. Most of them contain the reaction rates k_1 or k_3 or the inlet concentration c (or the parameters \bar{k}_1 , \bar{k}_3 , and \bar{c} or the system copy). Removing these components obviously violates the parameter space and results in an ideal

$$\begin{aligned}\langle x_1 - \bar{x}_2, x_2 - \bar{x}_2, k_1 - \bar{k}_1, k_2 - \bar{k}_2, k_3 - \bar{k}_3, c - \bar{c} \rangle \cap \\ \langle k_3\bar{k}_1^2 - k_1^2\bar{k}_3, k_3\bar{k}_1\bar{c} + k_1^2, k_1c - \bar{k}_1\bar{c}, k_3c + k_1, \bar{k}_3\bar{c} + \bar{k}_1, x_1 - c, x_2 - \bar{x}_2, k_2 - \bar{k}_2, \bar{x}_1 - \bar{c} \rangle.\end{aligned}$$

containing only two irreducible components. The second ideal still has generators that take only positive values in the whole parameter space. Thus, the only remaining component is the ideal corresponding to equal states and parameters, asserting that this system is globally identifiable and also globally observable.

5. Discussion

The problem of deciding global or local identifiability of a system has been addressed by viewing the parameters as additional state variables and testing the observability of these. In contrast to the ordinary observability problem, various kinds of state variables exist in the extended system that may be handled differently. Algebraic criteria for global and local identifiability, with or without known initial conditions, have been given. These can be tested for each individual physical parameter. For locally yet not globally identifiable or observable systems, the critical points in the state and parameter space can be computed as well. This information may be used to select appropriate initial conditions or input signals for identification experiments, such that these points are avoided. Furthermore, parameter constellations that prevent their identification can be computed in advance.

The approach used herein differs from algebraic methods for identifiability tests that eliminate the system state. While our method introduces additional variables, we can entirely avoid calculations in a differential ring. Nonetheless, computations in the ordinary or differential polynomial ring may require a large computational effort even for systems that appear very simple, as the expressions swell very quickly. Which criterion performs better may depend on the system itself as well as on the underlying algorithms used. In addition, the monomial ordering as well as the ranking of the differential monomials have a high impact on the computation time and size of the intermediate results. No comparison of the different approaches has been carried out until this point.

Currently, the manageable systems must allow a state-space representation with a polynomial vector field in both the state and the parameters, as opposed to the differential-

algebraic methods that naturally support rational vector fields, and can thus handle a greater system class. One can possibly overcome this limitation.

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