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Algebraic identifiability of partial differential equation models

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Abstract

Differential equation models are crucial to scientific processes across many disciplines, and the values of model parameters are important for analyzing the behaviour of solutions. Identifying these values is known as a parameter estimation, a type of inverse problem, which has applications in areas that include industry, finance and biomedicine. A parameter is called globally identifiable if its value can be uniquely determined from the input and output functions. Checking the global identifiability of model parameters is a useful tool when exploring the well-posedness of a given model. This problem has been intensively studied for ordinary differential equation models, where theory, several efficient algorithms and software packages have been developed. A comprehensive theory for PDEs has hitherto not been developed due to the complexity of initial and boundary conditions. Here, we provide theory and algorithms, based on differential algebra, for testing identifiability of polynomial PDE models. We showcase this approach on PDE models arising in the sciences.

Keywords: mathematical biology, structural parameter identifiability, input–output equations, nonlinear PDE models

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1. Introduction

Differential equations form the bedrock of numerous scientific and engineering models, particularly in the realms of biological and chemical interactions. Indeed, systems of ordinary and partial differential equations are integral to our understanding of such scientific phenomena. These models invariably incorporate time-varying dependent variables, input functions, and output functions, along with parameter vectors. Without loss of generality, parameters are positive scalars, which are independent of time, and whose values are often unknown. Parameter estimation or inference, which is an inverse problem, involves determining the unknown parameter values from observations. Parameter estimation is crucial to predicting behaviour from models, ranging from systems biology [1], chemical reactions in development [2], wave propagation in species interactions [3] and response to cell dynamics [4] and tumour response to treatment [5].

There are different notions of parameter identifiability for differential equation models [6]. A parameter is called *globally structurally identifiable* if its value can be uniquely determined from the input and output functions. As a result, checking the global structural identifiability of model parameters is a useful tool when exploring the well-posedness for a given model. If a parameter takes finitely many values, it is called locally identifiable. A parameter that is neither globally, nor locally identifiable, is called unidentifiable. In this paper, we only consider global identifiability and, for brevity, use the notation identifiable for global identifiability. Given a model with observables, the *parameter identifiability problem* is determining whether the parameters are identifiable.

For ordinary differential equation (ODE) models, the parameter identifiability problem has been extensively studied. Various approaches have emerged in areas ranging from control theory and dynamical systems (e.g. Taylor series approximations) to computational algebraic geometry and differential algebra. Starting from Ritt [7], several theoretical results and algorithms have been developed within the last decades. The Rosenfeld–Gröbner algorithm and Gröbner bases are the two crucial concepts that underpin existing identifiability algorithms. Based on these, several software have been designed to test identifiability, e.g. DAISY [8], SIAN [9], COMBOS [10], structural identifiability toolbox [11], and StructuralIdentifiability.jl [12]. An increase in the availability of spatio-temporal data enables the investigation of parameter values in PDE models. An approach using numerical algebraic geometry was introduced in [13].

A key aim of this work is to adapt and extend the successful algebraic approaches for studying ODE identifiability to spatial systems. PDEs are inherently more complex than ODEs. There are additional challenges associated with the boundary conditions. With the exception of the work [14–18], there is no systematic study of PDE identifiability, to the best of our knowledge. One of the first articles to generalize the differential algebra approach from the ODE to the PDE case, using a system of reaction–diffusion equations, is [14]. In [15], the authors investigate the identifiability and estimation of parameters of a chikungunya epidemic transmission model. Structural identifiability of age-structured PDE models using a differential algebra framework has been studied in [16]. Structural and practical identifiability of PDE models of fluorescence recovery after photobleaching has been studied in [17]. In [18], the authors present a differential algebra approach to structural identifiability analysis on partially observed linear reaction-advection-diffusion PDE models.

We extend the identifiability problem to spatio-temporal models

$$\Sigma = \begin{cases} \partial_t \mathbf{v} = \mathbf{f}\left(\mathbf{k}, \mathbf{w}, \mathbf{v}, \partial_x \mathbf{v}, \ldots, \partial_x^h \mathbf{v}\right) \\ \mathbf{y} = \mathbf{g}\left(\mathbf{k}, \mathbf{w}, \mathbf{v}, \partial_x \mathbf{v}, \ldots, \partial_x^h \mathbf{v}\right), \end{cases} \tag{1}$$

which have broad applications in applied mathematics. Here $\mathbf{w}(x,t)$, $\mathbf{v}(x,t)$, $\mathbf{y}(x,t)$, and $\mathbf{k}$ are vectors of inputs, state variables, outputs, and constant parameters, respectively and $\mathbf{f}$ and $\mathbf{g}$ are vectors of rational functions. We present an algebraic approach for the PDE identifiability problem, focusing on models arising in applied mathematics. Our main results state that for a given model of the form System (1), one can construct certain differential polynomials equations called Input Output (IO) equations such that the identifiability of the parameters can be obtained from the identifiability of the coefficients of the IO-equations (theorem 1), and that the coefficients of the IO-equations are identifiable if their Wronskian is nonsingular (proposition 1). Based on our results, we present two algorithms (for IO-identifiability and strong identifiability), with implementation in MAPLE for our illustrating examples, that provide a sufficient condition for solving the PDE identifiability problem. The main steps of our algorithms are the following:

- calculating IO equations of the PDE model (Step 1 in algorithms 1 and 2),
- checking if the parameters can be uniquely determined from the coefficients of the IO-equations (Step 3 in algorithm 1, Steps 2 & 3 in algorithm 2), and
- verifying that the coefficients of the IO-equations are themselves identifiable (Step 3 in algorithm 1, Step 4 in algorithm 2).

In the ODE case, there is a key subtlety: even for generic initial conditions, the coefficients of the IO-equations are not always identifiable, see e.g. [6, example 2.14]. Surprisingly, this subtlety does not occur in PDEs with generic initial/boundary conditions, as we prove in theorem 1 and exploit in algorithm 1.

Initial and boundary conditions in practical examples are not necessarily generic (see the ODE case [19, 20]), which adds an additional layer of difficulty. To account for these conditions, the last step of our method finds potential linear dependencies between the monomials present in the input–output equations corresponding to the PDE models. The linear dependencies are then tested by computing the Wronskian of the monomials and using differential algebra tools to determine if the Wronskian is non-singular. Using the Rosenfeld–Gröbner algorithm [21], we compute the normal form of the determinant of the Wronskian with respect to the differential ideal of the model. We then use the initial and boundary conditions of the model in order to refute the vanishing of the determinant (see proposition 1).

We demonstrate these results in algorithm 2, for testing the identifiability of standard models arising in applied mathematics. We consider different types of PDEs (parabolic, elliptic and hyperbolic), with a particular focus on parabolic PDEs that arise in mathematical biology. We show that a scalar reaction–diffusion equation, Fisher's equation, the coupled reaction–diffusion equations system, and a reaction–diffusion system [22, 23] are all identifiable. We also demonstrate the wider applicability of this framework on Laplace's equation (elliptic) and the wave equation (hyperbolic). In example 14, we show that following our symbolic-computation based algorithm directly could be too demanding on the computational resources. We demonstrate how numeric computation with random values of parameters gives evidence for identifiability at a generic point in reasonable computing time.

The organization of the paper is as follows. Section 2 outlines the preliminaries on differential algebra, detailing precise definitions and required results. Section 3 presents our results, offering the theoretical foundation for our PDE identifiability procedure using the Wronskian and generalizing the literature on ODE identifiability. Section 4 provides our two identifiability algorithms. In section 5, we showcase algorithm 2 on the above suite of PDE models arising in mathematical biology.

2. Differential equations to differential algebra

We start the preliminaries by recalling differential polynomials, which provide a general framework for polynomial PDEs. We illustrate the definitions with simple examples. While some examples have a clear physical meaning, their main purpose is to clarify the definitions.

Definition 1 (Ring of differential polynomials). (i) A *differential ring* (R, Δ) is a commutative ring with a set $\Delta = \{\partial_1, \ldots, \partial_m\}$ of pairwise-commuting derivations $\partial_i : R \to R$, that is, maps such that, for all $a, b \in R$, $\partial_i(a+b) = \partial_i(a) + \partial_i(b)$ and $\partial_i(ab) = \partial_i(a)b + a\partial_i(b)$.

(ii) A differential ring that is a field is called a *differential field*.

(iii) For a differential field K, the *ring of differential polynomials* in the variables $x_1, \ldots, x_n$ over a differential field K is the polynomial ring in infinitely many variables

$$K[\partial_1^{n_1} \cdots \partial_m^{n_m} x_j \mid n_i \geqslant 0, 1 \leqslant j \leqslant n]$$

with the derivations extended from K by

$$\partial_i\left(\partial_1^{n_1} \cdots \partial_i^{n_i} \cdots \partial_m^{n_m}(x_j)\right) := \partial_1^{n_1} \cdots \partial_i^{n_i+1} \cdots \partial_m^{n_m}(x_j).$$

This differential ring is denoted by $K\{x_1, \ldots, x_n\}$.

Example 1. Consider the case of one spatial variable x and one temporal variable t. We then have two derivations, ∂_x and ∂_t and $\Delta = \{\partial_x, \partial_t\}$. Complex-valued functions of x and t meromorphic on a domain is an example of a differential field K. If we have a PDE in one dependent variable u with derivations Δ and coefficients in K, then we consider this ring of differential polynomials:

$$K\{u\} = K\left[u, \partial_x u, \partial_t u, \partial_x\partial_t u, \partial_x^2 u, \partial_t^2 u, \ldots\right] = K\left[u, u_x, u_t, u_{xt}, u_{xx}, u_{tt}, \ldots\right].$$

Definition 2 (Strong identifiability). Let $\mathbb{K}$ be one of the fields $\mathbb{R}$ and $\mathbb{C}$. We fix a domain $\mathcal{D}$ in $\mathbb{K}^m$ on which a PDE system will be defined. We will consider a PDE system in n variables $\mathbf{v} = (v_1, \ldots, v_n)$ and, for each $1 \leqslant i \leqslant n$, we fix a class $\mathcal{C}_i$ of function in $\mathcal{D}$ where the solutions for v_i will be sought. The requirements on functions from $\mathcal{C}_i$ may involve, for example, regularity conditions (e.g. twice or infinitely differentiable) or boundary conditions on $\partial\mathcal{D}$.

Now we consider a system of PDEs in $\mathcal{D}$ of the form

$$\mathbf{F}(\mathbf{k}, \mathbf{v}) = 0, \tag{2}$$

where $\mathbf{F} = (F_1, \ldots, F_s)$ and $F_1, \ldots, F_s \in \mathbb{K}(\mathbf{k})\{\mathbf{v}\}$ are differential polynomials in $\mathbf{v}$ with coefficients that are rational functions in the scalar parameters $\mathbf{k} = (k_1, \ldots, k_\ell)$. Let us fix a domain $\Omega \subset \mathbb{K}^\ell$, which will play the role of the domain for the parameters (in our examples, if Ω is not specified, we will assume that $\Omega = \mathbb{K}^\ell$). Furthermore, we fix outputs $\mathbf{y} = (y_1, \ldots, y_r)$ defined by given formulas

$$y_i = \frac{G_i(\mathbf{k}, \mathbf{v})}{Q(\mathbf{k}, \mathbf{v})}, \quad 1 \leqslant i \leqslant r,$$

where $G_1, \ldots, G_r, Q \in \mathbb{K}(\mathbf{k})\{\mathbf{v}\}$. We will say that a rational function $h(\mathbf{k}) \in \mathbb{K}(\mathbf{k})$ is *strongly identifiable* if, for all $\mathbf{k}_1, \mathbf{k}_2 \in \Omega$ and all $\mathbf{v}_1, \mathbf{v}_2 \in \mathcal{C}_1 \times \ldots \times \mathcal{C}_n$ such that $\mathbf{F}(\mathbf{k}_1, \mathbf{v}_1) = \mathbf{F}(\mathbf{k}_2, \mathbf{v}_2) = 0$, we have

$$\mathbf{y}(\mathbf{k}_1, \mathbf{v}_1) = \mathbf{y}(\mathbf{k}_2, \mathbf{v}_2) \implies h(\mathbf{k}_1) = h(\mathbf{k}_2).$$

Example 2. Consider the PDE

$$u_t = a u_x, \tag{3}$$

$\Omega = \mathbb{R} \setminus \{0\}$, and $\mathcal{C}$ be the C^∞-functions f of x and t on the domain $\mathcal{D} = [0,1] \times [0,1]$ such that $f(0,t) = \mathrm{e}^t$. A calculation shows that any solution of (3) is equal to $\mathrm{e}^{t + \frac{x}{a}}$. To check the strong identifiability of $\mathbf{k} = a$, consider arbitrary values a_1 and a_2 from Ω and the corresponding solutions $\mathbf{v}_1 = \mathrm{e}^{t + \frac{x}{a_1}}$ and $\mathbf{v}_2 = \mathrm{e}^{t + \frac{x}{a_2}}$ from $\mathcal{C}$. If

$$\mathbf{v}_1 = \mathrm{e}^{t + \frac{x}{a_1}} = \mathbf{v}_2 = \mathrm{e}^{t + \frac{x}{a_2}}$$

as functions of x and t, that is, for all $(x,t) \in \mathcal{D}$, then $a_1 = a_2$, and so a is strongly identifiable. If we change the boundary condition to $f(0,t) = 1$, then the solution would be $u(x,t) = 1$, and we see that the parameter a is not strongly identifiable for this choice of $\mathcal{C}$.

Remark 1. While the definition above is very general and stated in natural analytic terms, some of its properties make it challenging to use it in practice: First, since it allows for arbitrary function classes and arbitrary polynomial PDEs, a complete constructive approach to verifying this property seems to be out of reach at the moment. Nevertheless, we will show that strong identifiability can be established in a variety of practical cases by a uniform approach (see section 5).

Second, a system that is 'almost always' identifiable can become nonidentifiable according to this definition because of some special degenerate cases. For example, a parameter k in the ODE model $x'(t) = kx(t)$ with output $y(t) = x(t)$ will be considered nonidentifiable because the zero solution $x(t) = 0$ does not distinguish between different parameter values. However, as long as $x(t)$ is nonzero, the value of k is uniquely determined. The standard mitigation of this issue in the ODE case is to restrict the discussion to generic solutions. The problem is that because of significantly more involved conditions on the existence and uniqueness of solutions of PDEs, the topology (and thus the notion of genericity) of the solution space of a PDE system may be much more involved even if the function classes $\mathcal{C}_1, \ldots, \mathcal{C}_n$ are infinitely differentiable functions subject to some boundary conditions.

Therefore, to obtain more refined results in a more restricted context, we will give another definition, which is a direct analogue of the notion of algebraic identifiability in the ODE case [24, section 2.2]. Note that, in the ODE case, this definition is equivalent to the analytic one [6, proposition 3.4], and we expect a similar equivalence result to hold in the PDE case (perhaps in the class of power series or analytic solutions).

We will recall some relevant notions from differential algebra.

Definition 3 (Differential ideals). An ideal I of a differential ring (R, Δ) is called a *differential ideal* if, for all $a \in I$ and $\partial \in \Delta$, $\partial(a) \in I$. For $F \subset R$, the smallest differential ideal containing the set F is denoted by $[F]$.

For an ideal I and set S in a ring R, we denote S^∞ to be the multiplicatively closed subset of R generated by S and

$$I\colon S^\infty = \{r \in R \mid \exists a \in S^\infty : ar \in I\}.$$

The set $I : S^\infty$ is also an ideal in R. If $S = \{a\}$ for some $a \in R$, we also denote $I : S^\infty$ by $I : a^\infty$.

Example 3. Consider the PDE $u_x = u_t$. It can be viewed as a differential polynomial—see example 1. The corresponding differential ideal is generated as a polynomial ideal by

$$u_x - u_t, u_{xx} - u_{tx}, u_{xt} - u_{tt}, \ldots, \tag{4}$$

knowing that $u_{tx} = u_{xt}$, etc. The meaning behind (4) is that, if u is a solution of $u_x = u_t$, then it satisfies all of these relations (4). For the reverse direction, see definition 4 and example 4.

As mentioned in the introduction, we will mostly focus on evolutionary PDEs. More precisely, we will have one distinguished derivation ∂_t with respect to the time and one or several spatial derivations $\partial_1, \ldots, \partial_m$, and we will consider systems of the form

$$\Sigma = \begin{cases} \partial_t \mathbf{v} = \frac{\mathbf{f}(\mathbf{k},\mathbf{v},\mathbf{w})}{Q(\mathbf{k},\mathbf{v},\mathbf{w})} \\ \mathbf{y} = \frac{\mathbf{g}(\mathbf{k},\mathbf{v},\mathbf{w})}{Q(\mathbf{k},\mathbf{v},\mathbf{w})}, \end{cases} \tag{5}$$

where $\mathbf{v}$ and $\mathbf{w}$ are the state and input variables of the model, $\mathbf{y}$ are outputs, $\mathbf{k}$ are scalar parameters, and $\mathbf{f}, \mathbf{g}, Q$ are differential polynomials in $\mathbf{v}, \mathbf{w}$ with coefficients in $\mathbb{C}(\mathbf{k})$ of order zero with respect to ∂_t. Note that we have focused on complex numbers to unlock powerful algebraic tools we will use, and identifiability over complex numbers implies identifiability over reals. Now we will give a formal definition of what generic solution of (5) is and then give our second definition of identifiability.

Definition 4 (Generic solution). Given Σ as in (5), we define the differential ideal of Σ as

$$I_\Sigma = [Q\partial_t \mathbf{v} - \mathbf{f}, Q\mathbf{y} - \mathbf{g}] : Q^\infty \subset \mathbb{C}(\mathbf{k})\{\mathbf{v}, \mathbf{y}, \mathbf{w}\}.$$

In the same way as [6, lemmas 3.1 and 3.2], one can show that I_Σ is a prime ideal and

$$I_\Sigma \cap \mathbb{C}(\mathbf{k})\{\mathbf{w}\}\left[\partial_1^{i_1} \ldots \partial_m^{i_m} \mathbf{v},\ i_1, \ldots, i_m \geqslant 0\right] = \{0\}. \tag{6}$$

Let K be a differential field containing $\mathbb{C}(\mathbf{k})$. We say that a tuple $(\hat{\mathbf{v}}, \hat{\mathbf{y}}, \hat{\mathbf{w}})$ is a *generic solution* of Σ in K if all components of the tuple belong to K and a differential polynomial relation $p = 0$ with coefficients in $\mathbb{C}(\mathbf{k})$ holds among the tuple entries if and only if $p \in I_\Sigma$. In particular, since I_Σ is prime, we can consider the field of fractions of R/I_Σ, which we denote by $\mathcal{F}$. Then the images of $\mathbf{v}, \mathbf{y}, \mathbf{w}$ in $\mathcal{F}$ form a generic solution of (5) (in $\mathcal{F}$).

Example 4. Let Σ be the PDE $u_x = u_t$. The function $u(x,t) = 0$ is a solution of the PDE but is not a generic solution. The latter is because $u(x,t) = 0$ tautologically satisfies the relation $u = 0$, which does not belong to the differential ideal I_Σ. Another example of a non-generic solution is $u(x,t) = x + t$. This is because it satisfies $u_{xx} = 0$, which does not belong to I_Σ. An example of a generic solution would be $f(x+t)$, where f is a hypertranscendental function, e.g. the gamma function Γ.

Definition 5 (Identifiability). In the notation of the previous definition, we say that a parameter $k_i \in \mathbf{k}$ (or, more generally, a rational function of parameters) is *identifiable* if

$$k_i \in \mathbb{C}\langle \hat{\mathbf{y}}, \hat{\mathbf{w}} \rangle,$$

where $\mathbb{C}\langle \hat{\mathbf{y}}, \hat{\mathbf{w}} \rangle$ is the smallest field extension of $\mathbb{C}$ containing $\hat{\mathbf{y}}, \hat{\mathbf{w}}$ and their derivatives.

Example 5. Consider the PDE $u_t = a u_x$, without any initial/boundary conditions at this point. The function $f(x,t) = \Gamma(\frac{x}{a} + t)$ is a generic solution of this equation (see example 4). Moreover, we have $a = \frac{f_t}{f_x}$, and so $a \in \mathbb{C}\langle f \rangle$ and a is identifiable.

Note that $a \notin \mathbb{C}\langle g \rangle$ for such solutions g of $u_t = a u_x$ that $g_x = 0$. However, these are not generic solutions because u_x does not belong to the differential ideal generated by u_t - $a u_x$.

3. Results

We present our main theoretical results in this section. We also include toy examples to clarify the statements of our results. These examples do not necessarily have any physical meaning but are helpful to follow the theory.

3.1. Identifiability for generic solutions

We will prove that, unlike the ODE case, all of the identifiable functions of parameters can be read off from particular relations between the input and output variables called input–output equations. Below we recall some necessary notions and constructions from constructive differential algebra.

Definition 6 (Differential rankings and characteristic sets). (i) A *differential ranking* on $K\{x_1, \ldots, x_n\}$ is a total order $>$ on

$$X := \{\partial_1^{n_1} \cdots \partial_n^{n_m}(x_j) \mid n_i \geqslant 0, 1 \leqslant j \leqslant n\}$$

satisfying:

- for all $x \in X$ and $\partial \in \Delta$, $\partial(x) > x$ and
- for all $x, y \in X$ and $\partial \in \Delta$, if $x > y$, then $\partial(x) > \partial(y)$.

It can be shown that a differential ranking on $K\{x_1, \ldots, x_n\}$ is always well-ordered.

(ii) For $f \in K\{x_1, \ldots, x_n\} \backslash K$ and differential ranking $>$,
- $\mathrm{lead}(f)$ is the element of X appearing in f that is maximal with respect to $>$.

- The *leading coefficient* of f considered as a polynomial in $\mathrm{lead}(f)$ is denoted by $\mathrm{in}(f)$ and called the *initial* of f.
- The *separant* of f is $\frac{\partial f}{\partial\,\mathrm{lead}(f)}$, the partial derivative of f with respect to $\mathrm{lead}(f)$.
- The *rank* of f is $\mathrm{rank}(f) = \mathrm{lead}(f)^{\deg_{\mathrm{lead}(f)} f}$.
- For $S \subset K\{x_1,\ldots,x_n\}\backslash K$, the set of *initials* and *separants* of S is denoted by H_S.
- For $g \in K\{x_1,\ldots,x_n\}\backslash K$, say that $f < g$ if $\mathrm{lead}(f) < \mathrm{lead}(g)$ or $\mathrm{lead}(f) = \mathrm{lead}(g)$ and $\deg_{\mathrm{lead}(f)} f < \deg_{\mathrm{lead}(g)} g$.

(iii) For $f, g \in K\{x_1,\ldots,x_n\}\backslash K$, f is said to be reduced w.r.t. g if no proper derivative of $\mathrm{lead}(g)$ appears in f and $\deg_{\mathrm{lead}(g)} f < \deg_{\mathrm{lead}(g)} g$.

(iv) A subset $\mathcal{A} \subset K\{x_1,\ldots,x_n\}\backslash K$ is called *autoreduced* if, for all $p \in \mathcal{A}$, p is reduced w.r.t. every element of $\mathcal{A} \setminus \{p\}$. One can show that every autoreduced set is always finite.

(v) Let $\mathcal{A} = \{A_1,\ldots,A_r\}$ and $\mathcal{B} = \{B_1,\ldots,B_s\}$ be autoreduced sets such that $A_1 < \ldots < A_r$ and $B_1 < \ldots < B_s$. We say that $\mathcal{A} < \mathcal{B}$ if

- $r > s$ and $\mathrm{rank}(A_i) = \mathrm{rank}(B_i)$, $1 \leqslant i \leqslant s$, or
- there exists q such that $\mathrm{rank}(A_q) < \mathrm{rank}(B_q)$ and, for all i, $1 \leqslant i < q$, $\mathrm{rank}(A_i) = \mathrm{rank}(B_i)$.

(vi) An autoreduced subset of the smallest rank of a differential ideal $I \subset K\{x_1,\ldots,x_n\}$ is called a *characteristic set* of I. One can show that every non-zero differential ideal in $K\{x_1,\ldots,x_n\}$ has a characteristic set. Note that a characteristic set does not necessarily generate the ideal.

(vii) For elements $r_1,\ldots,r_n$ is a differential ring (R,Δ), the Wronskian matrix $\mathrm{Wr}_\partial(r_1,\ldots,r_n)$ with respect to a given $\partial \in \Delta$ is the matrix

$$\begin{pmatrix} r_1 & \ldots & r_n \\ \partial r_1 & \ldots & \partial r_n \\ \vdots & \ddots & \vdots \\ \partial^{n-1} r_1 & \ldots & \partial^{n-1} r_n \end{pmatrix}.$$

Example 6. Consider the following PDE system in two dependent variables u and v:

$$\begin{cases} u_t = au_x + cv^2, \\ v_t = bu_{xx} \end{cases} \tag{7}$$

with unknown scalar parameters a , b and c. We then consider the ring of differential polynomials

$$\mathbb{C}(a,b,c)\{u,v\} = \mathbb{C}(a,b,c)[u,v,u_x,v_x,u_t,v_t,\ldots].$$

One, useful in this paper, way to rank the elements of the set $u,v,u_x,v_x,u_t,v_t,\ldots$ is to declare that $u > v$ and any derivative of u is ranked higher than any derivative of v. So, we have the following order

$$v < v_x < v_t < v_{xx} < v_{tx} < v_{tt} < \ldots < u < u_x < u_t < u_{xx} < u_{tx} < u_{tt} < \ldots. \tag{8}$$

This ranking is called an *elimination ranking*. With respect to this ranking, the leader, initial and separant of

$$u_x - au_x - cv^2 \tag{9}$$

are u_x, 1, and 1, respectively. On the other hand, if we switch u and v in (8):

$$u < u_x < u_t < u_{xx} < u_{tx} < u_{tt} < \ldots < v < v_x < v_t < v_{xx} < v_{tx} < v_{tt} < \ldots, \tag{10}$$

the leader, initial, and separant of (9) will be v, $-c$, and $-2cv$, respectively. Furthermore, under this ranking,

$$u_x - au_x - cv^2 < v_t - bu_{xx}$$

because $v < v_t$. Under this ranking, the system (7) is not autoreduced because the second equation is not reduced with respect to the first one (v_x and v^2 appear there, respectively). However, it is autoreduced with respect to the ranking (8), although this autoreduced set is not a characteristic set of the corresponding differential ideal. Indeed, a computation in MAPLE shows that

$$u_x - au_x - cv^2,\ v_t - bu_{xx},\ v_{tt} - 2bcvv_{xx} - 2bcv_x^2 - av_{tx} \tag{11}$$

is a characteristic set (w.r.t. ranking (8)) – see the second bullet in item (v) of definition 6. The Wronskian matrix of v_{xx}, v_x^2, and v_{tx} with respect to ∂_t is

$$\begin{pmatrix} vv_{xx} & v_x^2 & v_{tx} \\ v_tv_{xx} + vv_{xxt} & 2v_xv_{xt} & v_{ttx} \\ v_{tt}v_{xx} + 2v_tv_{xxt} + vv_{xxtt} & 2v_{xt}^2 + 2v_xv_{xtt} & v_{tttx} \end{pmatrix}.$$

Definition 7 (IO-equations). Given a differential ranking on the differential variables $\mathbf{y}$ and $\mathbf{w}$, the *IO-equations* are defined as the monic characteristic presentation of the prime differential ideal $I_\Sigma \cap \mathbb{C}(\mathbf{k})\{\mathbf{y}, \mathbf{w}\}$ with respect to this ranking (see [25, definition 6 and section 5.2] for more details). For each differential ranking, such a monic characteristic presentation is unique [26, theorem 3].

Example 7. Continuing example 6, let $v = \mathbf{y}$, so v is the output variable (no input variables), so choosing ranking (8). Then, intersecting (11) with $\mathbb{C}(a, b, c)\{v\}$, we obtain the following IO-equation of system (7):

$$v_{tt} - 2bcvv_{xx} - 2bcv_x^2 - av_{tx}. \tag{12}$$

Now we are ready to state the main result of this section, namely, that all the identifiable functions can be read off the coefficients of the IO-equations. Interestingly, the corresponding statement is not true for ODEs [25, example 2].

Theorem 1 (see [25, theorems 1 & 2]). *For a model Σ of the form (5), the identifiable functions in $\mathbb{C}(\mathbf{k})$ form a subfield, and this subfield is generated by the coefficients of any set of IO-equations of the model.*

Example 8. By theorem 1, it follows from example 7 that the set of identifiable functions of model (7) with output v is the field $\mathbb{C}(a, bc)$. In particular, a is identifiable and neither b nor c are identifiable but bc is identifiable.

Remark 2. Note that using theorem 1, one obtains identifiability of the coefficients C of the IO-equations $F_j(\mathbf{w}, \mathbf{y})$, $1 \leqslant j \leqslant s$, considered as differential polynomials in $\mathbf{w}, \mathbf{y}$. Elements of C are in fact the generators of the field of identifiable functions. For each parameter k_i in $\mathbf{k}$, one can check its identifiability by verifying whether $k_i \in \mathbb{Q}(C)$. This can be reduced to the ideal membership problem as described in [27, section 1.3] (for a randomized version, see [12, theorem 3.3]). The MAPLE code [28] has been implemented in [29] for testing this ideal membership.

Before proving theorem 1, we will proceed with some preparation. Consider a PDE model Σ as in (1), its prime differential ideal I_Σ, and the corresponding field of fractions $\mathcal{F}$ (see definition 4). Since I_Σ is stable under ∂_t and ∂_x, the derivations ∂_t and ∂_x can be transferred to $\mathcal{F}$ in a natural way.

Definition 8. We will call an element $c \in \mathcal{F}$ a *constant* if $\partial_t c = \partial_x c = 0$.

The key difference with the ODE case will be the following lemma.

Lemma 1. *If $c \in \mathcal{F}$ and $\partial_x(c) = 0$, then $c \in \mathbb{C}(\mathbf{k})$. In particular, the set of constants of $\mathcal{F}$ is $\mathbb{C}(\mathbf{k})$.*

Proof. Let $c = \frac{p}{q} \in \mathcal{F}$ be such $\partial_x(c) = 0, p, q \in R = \mathbb{C}(\mathbf{k})\{\mathbf{v}, \mathbf{y}, \mathbf{w}\}$ are coprime and at least one of them does not belong to $\mathbb{C}(\mathbf{k})$. There exists a positive integer N such that, using equations (1) and their derivatives, we can replace $Q^N p$ and $Q^N q$ by elements of $\mathbb{C}(\mathbf{k})\{\mathbf{w}\}[\partial_x^i \mathbf{v},\ i \geqslant 0]$ equivalent to $Q^N p$ and $Q^N q$ modulo I_Σ and, thus, yielding the same element of $\mathcal{F}$. By (6), $\mathcal{F}$ has a subfield isomorphic to the field of rational functions

$$\mathcal{F}_0 := \mathbb{C}(\mathbf{k}) \langle \mathbf{w} \rangle \left(\partial_x^i \mathbf{v},\ i \geqslant 0 \right),$$

and $\frac{p}{q}$ belongs to this subfield. With respect to ∂_x, the field $\mathcal{F}_0$ is isomorphic to the field of differential rational functions over $\mathbf{k}$ in infinitely many variables $\mathbf{v}, \mathbf{w}, \partial_t \mathbf{w}, \partial_t^2 \mathbf{w}, \ldots$. Since the constants of a field of differential rational functions are exactly the constants of the ground field, we deduce that $\frac{p}{q} \in \mathbb{C}(\mathbf{k})$. □

Lemma 2. *Let Δ be a finite set of derivations, $L \subset K$ differential fields, and X a finite set of variables. Let P be a prime non-zero differential ideal of $K\{X\}$ such that the ideal generated by P in $\overline{K}\{X\}$ is prime, where $\overline{K}$ is the algebraic closure of K. If $\mathcal{C}$ is a monic characteristic presentation of P, then the field of definition of P over L is the field extension of L generated by the coefficients of $\mathcal{C}$.*

Proof. *Mutatis mutandis* proof of [25, proposition 2]. □

Corollary 1 (see [25, corollary 1]). *If $\mathcal{C}$ is a monic characteristic presentation of the prime differential ideal $J := I_\Sigma \cap \mathbb{C}(\mathbf{k})\{\mathbf{y}, \mathbf{w}\}$, then field of definition of J over $\mathbb{C}$ is generated over $\mathbb{C}$ by the coefficients of $\mathcal{C}$.*

Proof. This follows from lemma 2 because the differential ideal generated by J in $\overline{\mathbb{C}(\mathbf{k})}\{\mathbf{y}, \mathbf{w}\}$ is prime. □

Lemma 3 (see [25, lemma 1]). *Consider a polynomial $P \in I_\Sigma \cap \mathbb{C}(\mathbf{k})\{\mathbf{y}, \mathbf{w}\}$ with at least one of the coefficients being one. If there is no element in $I_\Sigma \cap \mathbb{C}(\mathbf{k})\{\mathbf{y}, \mathbf{w}\}$ whose support is a subset of the support of P, then all coefficients of P are identifiable.*

Proof. We write $P = m_0 + \sum_{i=1}^{\ell} c_i m_i$, where $m_0, \ldots, m_\ell$ are monomials in

$$\left\{ \partial_t^i \partial_x^j \mathbf{y}, \partial_t^i \partial_x^j \mathbf{w} \mid i,j \geqslant 0 \right\}$$

and $c_1, \ldots, c_\ell \in \mathbb{C}(\mathbf{k})$. Let $(\hat{\mathbf{v}}, \hat{\mathbf{y}}, \hat{\mathbf{w}})$ be the generic solution of I_Σ. We consider the Wronskian

$$W(\hat{\mathbf{y}}, \hat{\mathbf{w}}) := \mathrm{Wr}\left(m_1\left(\hat{\mathbf{y}}, \hat{\mathbf{w}}\right), \ldots, m_\ell\left(\hat{\mathbf{y}}, \hat{\mathbf{w}}\right)\right)$$

with respect to ∂_x. If this Wronskian was singular, then, by [30, theorem 3.7], there would exist $a_1, \ldots, a_\ell \in F$ constant with respect to ∂_x so that

$$a_1 m_1\left(\hat{\mathbf{y}}, \hat{\mathbf{w}}\right) + \ldots + a_\ell m_\ell\left(\hat{\mathbf{y}}, \hat{\mathbf{w}}\right) = 0.$$

By lemma 1, $a_1, \ldots, a_\ell \in \mathbb{C}(\mathbf{k})$. This yields a nonzero element

$$a_1 m_1 + \ldots + a_\ell m_\ell \in I_\Sigma$$

with the support being a subset of the support of P. Thus, W is nonsingular. By taking the derivatives of $P(\hat{\mathbf{y}}, \hat{\mathbf{w}}) = 0$ of orders from 0 to $\ell - 1$ with respect to ∂_x, we obtain:

$$\begin{pmatrix} m_0(\hat{\mathbf{y}}, \hat{\mathbf{w}}) \\ \partial_x m_0(\hat{\mathbf{y}}, \hat{\mathbf{w}}) \\ \vdots \\ \partial_x^{\ell-1} m_0(\hat{\mathbf{y}}, \hat{\mathbf{w}}) \end{pmatrix} = W(\hat{\mathbf{y}}, \hat{\mathbf{w}}) \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_\ell \end{pmatrix}.$$

Viewing this as a nonsingular linear system in $c_1, \ldots, c_\ell$ over $\mathbb{C}\langle \hat{\mathbf{y}}, \hat{\mathbf{w}} \rangle$ and applying Cramer's rule, we deduce that each of $c_1, \ldots, c_\ell$ belongs to $\mathbb{C}\langle \hat{\mathbf{y}}, \hat{\mathbf{w}} \rangle$. □

Corollary 2. *If system (1) is of the form*

$$\Sigma = \begin{cases} \partial_t \mathbf{v} = \mathbf{f}\left(\mathbf{k}, \mathbf{w}, \mathbf{v}, \partial_x \mathbf{v}, \ldots, \partial_x^h \mathbf{v}\right) \\ \mathbf{y} = \mathbf{v}, \end{cases}$$

that is, all states are observable, then all coefficients of $\boldsymbol{f}$ *as polynomials in* $\mathbf{w}, \mathbf{v}, \partial_x \mathbf{v}, \ldots, \partial_x^h \mathbf{v}$ *are identifiable.*

Proof. It is sufficient to prove that polynomials $\partial_t \mathbf{v} - \mathbf{f}$ satisfy the condition of lemma 3. Assume that one of them, say $\partial_t v_1 - f_1$ does not. Therefore, there is a polynomial $g \in I_\Sigma$ with the support being a proper subset of the support of $\partial_t v_1 - f_1$. By cancelling $\partial_t v_1$, we obtain a $\mathbb{C}(\mathbf{k})$-linear combination $\tilde{g}$ of $\partial_t v_1 - f_1$ and g with the support being a subset of the support of f_1. Then $\tilde{g}$ is a nonzero element of $I \cap \mathbb{C}(\mathbf{k})\{\mathbf{w}\}[\partial_x^i \mathbf{v},\ i \geqslant 0]$, contradicting (6). □

We are now ready to prove our main result, theorem 1.

Proof of theorem 1. Let

$$S = \{c \in \mathbb{C}(\mathbf{k}) \mid c \text{ is identifiable}\} = \mathbb{C}(\mathbf{k}) \cap \mathbb{C}\langle \hat{\mathbf{y}}, \hat{\mathbf{w}} \rangle,$$

and so S is a subfield in $\mathbb{C}(\mathbf{k})$. Let $\mathcal{C}$ be a set of IO-equations of Σ and C the set of coefficients of $\mathcal{C}$. We will prove that $S = \mathbb{C}(C)$.

We first show that $S \subset \mathbb{C}(C)$. For this, let $c \in \mathbb{C}(\mathbf{k})$ be identifiable. We will show how the proof of [25, theorem 1] extends to PDEs to prove that $c \in \mathbb{C}(C)$. By corollary 1, the field of definition of $I_\Sigma \cap \mathbb{C}(\mathbf{k})\{\mathbf{y}, \mathbf{w}\}$ is equal to $\mathbb{C}(C)$. In particular, $I_\Sigma \cap \mathbb{C}(\mathbf{k})\{\mathbf{y}, \mathbf{w}\}$ is generated over $\mathbb{C}(\mathbf{k})$ by $I_\Sigma \cap \mathbb{C}(C)\{\mathbf{y}, \mathbf{w}\}$.

Since $c \in \mathbb{C}\langle \hat{\mathbf{y}}, \hat{\mathbf{w}} \rangle$, there exist $g \in \mathbb{C}\{\mathbf{y}, \mathbf{w}\} \setminus I_\Sigma$ and $h \in \mathbb{C}\{\mathbf{y}, \mathbf{w}\}$ such that $gc + h \in I_\Sigma$. Therefore, there exist $m_1, \ldots, m_r \in \mathbb{C}(\mathbf{k})\{\mathbf{y}, \mathbf{w}\}$ and $p_1, \ldots, p_r \in I_\Sigma \cap \mathbb{C}(C)\{\mathbf{y}, \mathbf{w}\}$ such that

$$gc + h = m_1 p_1 + \ldots + m_r p_r.$$

Now assume that $c \notin \mathbb{C}(C)$. By [31, theorem 9.29, p 117], there exists an automorphism σ on $\overline{\mathbb{C}(\mathbf{k})}$ that fixes $\mathbb{C}(C)$ pointwise, but does not fix c, i.e. $\sigma(c) \neq c$. Extend σ to $\overline{\mathbb{C}(\mathbf{k})}\{\mathbf{v}, \mathbf{y}, \mathbf{w}\}$ by letting σ fix $\mathbf{v}, \mathbf{y}$, and $\mathbf{w}$. We have in $\overline{\mathbb{C}(\mathbf{k})}\{\mathbf{v}, \mathbf{y}, \mathbf{w}\}$ that

$$\begin{aligned} (gc + h) - \sigma(gc + h) &= (m_1 p_1 + \ldots + m_r p_r) - \sigma(m_1 p_1 + \ldots + m_r p_r) \\ g(c - \sigma(c)) &= (m_1 - \sigma(m_1)) p_1 + \ldots + (m_r - \sigma(m_r)) p_r. \end{aligned} \tag{13}$$

Let $\overline{I_\Sigma}$ denote the differential ideal generated by I_Σ in $\overline{\mathbb{C}(\mathbf{k})}\{\mathbf{v}, \mathbf{y}, \mathbf{w}\}$. Since $\overline{I_\Sigma}$ is a prime differential ideal and the right-hand side of (13) belongs to $\overline{I_\Sigma}$, it follows that either $g \in \overline{I_\Sigma}$ or $c - \sigma(c) \in \overline{I_\Sigma}$. As $\sigma(c) \neq c$, we have that $c - \sigma(c)$ is a non-zero element of $\overline{\mathbb{C}(\mathbf{k})}$. Since $\overline{I_\Sigma}$ is a proper ideal, therefore $c - \sigma(c) \notin \overline{I_\Sigma}$. Therefore, $g \in \overline{I_\Sigma}$. Hence,

$$g \in \overline{I_\Sigma} \cap \mathbb{C}(\mathbf{k})\{\mathbf{v}, \mathbf{y}, \mathbf{w}\} = I_\Sigma,$$

contradicting the assumption on $g \notin I_\Sigma$.

For the proof of the converse, note that we have shown in lemma 1 that the set of constants of $\mathcal{F}$ coincides with $\mathbb{C}(\mathbf{k})$. Therefore, the assumption of [25, theorem 2] holds. So we follow the proof of [25, theorem 2] for PDEs.

Let $J := I_\Sigma \cap \mathbb{C}(\mathbf{k})\{\mathbf{y},\mathbf{w}\}$. Let $\mathcal{B}$ be the set of differential monomials in $\mathbf{y}$ and $\mathbf{w}$ indexed by $\mathbb{N}$ such that the indexing respects a ranking. Then $\mathcal{B}$ is a basis for $\mathbb{C}(\mathbf{k})\{\mathbf{y},\mathbf{w}\}$ as a vector space over $\mathbb{C}(\mathbf{k})$. Consider a basis $\mathcal{B}_J$ for J, as a $\mathbb{C}(\mathbf{k})$-subspace of $\mathbb{C}(\mathbf{k})\{\mathbf{y},\mathbf{w}\}$. Each element of $\mathcal{B}_J$ is a finite linear combination of the element of $\mathcal{B}$. Autoreduce $\mathcal{B}_J$ as a set of vectors expressed in the basis $\mathcal{B}$ and call it $\mathcal{B}_J'$. Note that $\mathcal{B}_J'$ is still a basis of J as a vector space. The field of definition of J over $\mathbb{C}$ is contained in the field generated by the coefficient of $\mathcal{B}_J'$ written as linear combinations of $\mathcal{B}$. Therefore, it is sufficient to prove that these coefficients are identifiable.

Let $P \in J$ be the differential polynomial corresponding to a member of $\mathcal{B}_J'$ of J. Let q be a polynomial whose support is a subset of P and whose monomials are linearly dependent modulo J over $\mathbb{C}(\mathbf{k})$. The representation of q in basis $\mathcal{B}$ can be reduced to zero by $\mathcal{B}_J$, however, q cannot be reduced to zero by P. Also, q reduced by P cannot be further reduced by other elements of $\mathcal{B}_J'$, as $\mathcal{B}_J'$ is a reduced basis. This proves that there is no q whose support is a subset of the support of P and whose support is linearly dependent. Therefore, by lemma 3, the coefficients of P are identifiable. □

3.2. *Identifiability for solutions with specified initial and boundary conditions*

In this section, we are in the setup of definition 2. Consider a PDE system of the form (2) and each $\mathcal{C}_i$ contained in the C^∞-functions on a domain $\mathcal{D}$. Fix a differential ranking such that any derivative of $\mathbf{v}$ is greater than any derivative of $\mathbf{y}$, and let

$$I_\Sigma = [C_1] : H_{C_1}^\infty \cap \ldots \cap [C_r] : H_{C_r}^\infty \tag{14}$$

be a decomposition computed by [26, section 4] or [32, algorithm 7.2] with respect to the differential ranking. For each i, $1 \leqslant i \leqslant r$, let

$$\widetilde{C}_i = C_i \cap \mathbb{C}(\mathbf{k})\{\mathbf{y}\}.$$

If the system Σ is as in (1), then, as we discussed, I_Σ is a prime differential ideal and, as a result, one can remove redundant components in (14) and obtain $r = 1$ and $\widetilde{C_1} \subset C_1 \subset I_\Sigma$, see [33, theorem 3.2.1]. If Σ is more general and I_Σ is not necessarily a prime differential ideal, consider the set $\widetilde{C} = \prod_{i=1}^r \widetilde{C}_i \subset I_\Sigma$. By dividing every element of $\widetilde{C}$ by an element of $\mathbb{C}(\mathbf{k})$, for every $c \in \widetilde{C}$, we pick a representation of the form

$$c = p_{0,c} + \sum_{j=1}^{q_c} a_{j,c} \cdot p_{j,c}, \tag{15}$$

where $p_0,\ldots,p_{q_c} \in \mathbb{C}\{\mathbf{y}\}$ and $a_1\ldots,a_{q_c} \in \mathbb{C}(\mathbf{k})$.

Remark 3. Such a grouping (15) is implemented in MAPLE in [28], the function `DecomposePolynomial`.

Example 9. Consider the PDE system

$$\begin{cases} u_t^2 = a v_x, \\ v_t = b u_x, \end{cases} \tag{16}$$

with output variable v. Since it is not of the form (1), we do not *a priori* know if the corresponding differential ideal is prime. We compute its decomposition in MAPLE and obtain that

$$C_1 = \left\{bu_t v_{xx} - 2v_x v_{tt},\ bu_x - v_t,\ -ab^2 v_{xx}^2 + 4v_x v_{tt}^2\right\},$$
$$C_2 = \left\{-av_x + u_t^2,\ bu_x - v_t,\ v_{tt},\ v_{xx}\right\},$$
$$C_3 = \left\{u_t,\ bu_x - v_t,\ v_{tt},\ v_x\right\}.$$

Intersecting these with $\mathbb{R}(a,b)\{v\}$, we obtain

$$\widetilde{C_1} = \left\{-ab^2 v_{xx}^2 + 4v_x v_{tt}^2\right\}, \tag{17}$$
$$\widetilde{C_2} = \left\{v_{tt},\ v_{xx}\right\}, \tag{18}$$
$$\widetilde{C_3} = \left\{v_{tt},\ v_x\right\}. \tag{19}$$

Then

$$\widetilde{C} = \left\{4v_x v_{tt}^4 - ab^2 v_{xx}^2 v_{tt}^2,\ 4v_x v_{xx} v_{tt}^3 - ab^2 v_{xx}^3 v_{tt},\ 4v_x^2 v_{tt}^3 - ab^2 v_{xx}^2 v_{tt} v_x,\ 4v_x^2 v_{tt}^2 v_{xx} - ab^2 v_{xx}^3 v_x\right\}.$$

Here we have

$$p_{1,1} = v_{xx}^2 v_{tt}^2, \quad a_{1,1} = -ab^2,$$
$$p_{1,2} = v_{xx}^3 v_{tt}, \quad a_{1,2} = -ab^2,$$
$$p_{1,3} = v_{xx}^2 v_{tt} v_x, \quad a_{1,3} = -ab^2,$$
$$p_{1,4} = v_{xx}^3 v_x, \quad a_{1,4} = -ab^2.$$

Proposition 1. *Let* $c \in \widetilde{C}$, *defined above. If, for all* $\widehat{\mathbf{k}} \in \Omega$ *and solutions* $(\widehat{\mathbf{v}}, \widehat{\mathbf{y}})$ *of (2) with the parameter values* $\widehat{\mathbf{k}}$, *there exists a point* $(t_0, x_0) \in \mathcal{D}$ *such that the matrix* $\mathrm{Wr}_\partial(p_{1,c}, \ldots, p_{q_c,c})|_{\mathbf{y}=\widehat{\mathbf{y}}, t=t_0, x=x_0}$, *where* $\partial \in \{\partial_x, \partial_t\}$, *is invertible, then*

- *all* $a_{1,c}, \ldots, a_{q_c,c}$ *are strongly identifiable.*
- *Moreover, let* $k_{i_1}, \ldots, k_{i_c}$ *be the parameters that explicitly appear in* $a_{1,c}, \ldots, a_{q_c,c}$. *If the 'coefficient map'*
  $$\varphi_c : (k_{i_1}, \ldots, k_{i_c}) \mapsto (a_{1,c}, \ldots, a_{q_c,c})$$
  is injective, then the parameters $k_{i_1}, \ldots, k_{i_c}$ *are strongly identifiable.*

Proof. Suppose that there exists j such that $a_{j,c}$ is not strongly identifiable according to definition 2. Let $\widehat{\mathbf{k}}_1, \widehat{\mathbf{k}}_2 \in \Omega$ and solutions $(\widehat{\mathbf{v}}_1, \widehat{\mathbf{y}}_1)$ and $(\widehat{\mathbf{v}}_2, \widehat{\mathbf{y}}_2)$ of (2) be such that

$$\widehat{\mathbf{y}}_1 = \widehat{\mathbf{y}}_2 \quad \text{but} \quad a_{j,c}\left(\widehat{\mathbf{k}}_1\right) \neq a_{j,c}\left(\widehat{\mathbf{k}}_2\right). \tag{20}$$

Consider any $\partial \in \{\partial_x, \partial_t\}$ and the square system of linear equations

$$\begin{cases} \sum_{j=1}^{q_c} a_{j,c} \cdot p_{j,c} = -p_{0,c} \\ \sum_{j=1}^{q_c} a_{j,c} \cdot \partial(p_{j,c}) = -\partial(p_{0,c}) \\ \quad\vdots \\ \sum_{j=1}^{q_c} a_{j,c} \cdot \partial^{q_c-1}(p_{j,c}) = -\partial^{q_c-1}(p_{0,c}) \end{cases} \tag{21}$$

in the unknowns $a_{1,c},\ldots,a_{q_c,c}$, whose matrix is $\mathrm{Wr}_\partial(p_{1,c},\ldots,p_{q_c,c})$. Assume that, for all $\widetilde{\mathbf{k}}\in\Omega$ and solutions $(\widetilde{\mathbf{v}},\widetilde{\mathbf{y}})$ of (2) with parameters $\widetilde{\mathbf{k}}$, there exists $(t_0,x_0)\in\mathcal{D}$ such that the matrix $\mathrm{Wr}_\partial(p_{1,c},\ldots,p_{q_c,c})|_{\mathbf{y}=\widetilde{\mathbf{y}},t=t_0,x=x_0}$ is invertible. Substituting $\widehat{\mathbf{y}}_1$ or $\widehat{\mathbf{y}}_2$ and the corresponding point

(t_0, x_0) into (21) and solving returns $\left(a_{1,c}(\widehat{\mathbf{k}}_1), \ldots, a_{q_c,c}(\widehat{\mathbf{k}}_1)\right)$ or $\left(a_{1,c}(\widehat{\mathbf{k}}_2), \ldots, a_{q_c,c}(\widehat{\mathbf{k}}_2)\right)$, respectively. By the first part of (20), these tuples are equal, which contradicts with the second part of (20).

For the proof of the second item, suppose that the coefficient map φ_c is injective. If k_{i_j} is not strongly identifiable, then there exist $\widehat{\mathbf{k}}_1, \widehat{\mathbf{k}}_2 \in \Omega$ and solutions $(\widehat{\mathbf{v}}_1, \widehat{\mathbf{y}}_1)$ and $(\widehat{\mathbf{v}}_2, \widehat{\mathbf{y}}_2)$ of (2) with parameter values $\widehat{\mathbf{k}}_1$ and $\widehat{\mathbf{k}}_2$ such that

$$\widehat{\mathbf{y}}_1 = \widehat{\mathbf{y}}_2 \quad \text{but} \quad \mathrm{proj}_{k_{i_j}}\left(\widehat{\mathbf{k}}_1\right) \neq \mathrm{proj}_{k_{i_j}}\left(\widehat{\mathbf{k}}_2\right).$$

Hence, by the injectivity of φ_c, there exists ℓ such that $a_{\ell,c}(\widehat{\mathbf{k}}_1) \neq a_{\ell,c}(\widehat{\mathbf{k}}_2)$, which contradicts the strong identifiability of $a_{\ell,c}$ established above. □

Example 10. Based on example 9, it remains to determine if at least one of the $p_{1,1}, \ldots, p_{1,4}$ does not vanish (these are 1×1 Wronskian determinants). Consider $p_{1,1}$. By computing remainders with respect to (17), (18), and (19), we obtain $ab^2 v_{xx}^4$, 0, and 0, respectively. Therefore, by proposition 1, we conclude that, if the class $\mathcal{C}$ is so that $v_{xx} \neq 0$ for at least one point in $\mathcal{D}$, then ab^2 is strongly identifiable. For example, if we specify a boundary condition $v(0,t) = 0$, then solutions of (16) are of the form

$$u(x,t) = c_1 + c_2 t, \quad v(x,t) = \frac{c_2^2 x}{a}, \tag{22}$$

where c_1 and c_2 are arbitrary constants. In this case, $v_{xx} = 0$, and proposition 1 is inconclusive. If we change the boundary condition to $v(0,t) = t^2$, then solutions of (16) are

$$u(x,t) = c_1 + c_2 t + \frac{2xt}{b}, \quad v(x,t) = t^2 + \frac{4x^3}{3ab^2} + \frac{2c_2 x^2}{ab} + \frac{c_2^2 x}{a}, \tag{23}$$

and so v_{xx} does not vanish at at least one point and ab^2 is strongly identifiable by proposition 1. The remainders of $p_{1,2}$, $p_{1,3}$, and $p_{1,4}$ with respect to (17), (18), and (19), are $\{p_{1,2}, 0, 0\}$, $\{p_{1,3}, 0, 0\}$, and $\{p_{1,4}, 0, 0\}$, respectively. Therefore, as above, the boundary condition $v(0,t) = 0$, which results in solutions (22), makes proposition 1 inconclusive too because the Wronskian vanishes at all points on solution (22). For the boundary condition $v(0,t) = t^2$, resulting in solutions (23), none of the $p_{1,2}$, $p_{1,3}$, or $p_{1,4}$ vanish identically at these solutions. So, by proposition 1, ab^2 is again strongly identifiable. Thus, all of $p_{1,1}$, $p_{1,2}$, $p_{1,3}$, and $p_{1,4}$ provide the same outcome regarding proposition 1 in this example.

4. Algorithms

The correctness of algorithms 1 and 2, which we present in this section, follows from theorem 1 and proposition 1, respectively.

Algorithm 1. Assessing identifiability in the sense of defintion 5.

Input A rational PDE system of the form

$$\begin{cases} \partial_t \mathbf{v} = \mathbf{f}\left(\mathbf{k}, \mathbf{w}, \mathbf{v}, \partial_x \mathbf{v}, \ldots, \partial_x^h \mathbf{v}\right) \\ \mathbf{y} = \mathbf{g}\left(\mathbf{k}, \mathbf{w}, \mathbf{v}, \partial_x \mathbf{v}, \ldots, \partial_x^h \mathbf{v}\right). \end{cases}$$

Output A list of generators of the field of identifiable functions of the system and, for each parameter, k_i whether it is identifiable or not.

(Step 1) Using `RosenfeldGroebner` with an elimination ranking $\mathbf{v} > \mathbf{y}, \mathbf{w}$, eliminate the variables $\mathbf{v}$ and obtain a set $\mathcal{S}$ of IO-equations of the input PDE system.

(Step 2) Let $\mathcal{C} \subset \mathbb{C}(\mathbf{k})$ be the set of the coefficients of $\mathcal{S}$.

(Step 3) **Return**:

- For the generators of the field of identifiable functions, the set $\mathcal{S}$. It can be additionally simplified using [28] by applying `FieldToIdeal` and then `FilterGenerators` (or [34, section 5]);
- For each $k_i \in \mathbf{k}$, the result of the test $k_i \in \mathbb{C}(\mathbf{k})$ (using, e.g. [27, section 1.3], see [28] for implementation).

Algorithm 2. Approach to establishing strong identifiability (defintion 2).

Input A system of rational PDEs of the form

$$\mathbf{F}(\mathbf{k}, \mathbf{v}) = 0, \quad \mathbf{y} = \mathbf{G}(\mathbf{k}, \mathbf{v}).$$

together with some set of requirements $\mathcal{R}$ (regularity, boundary conditions, etc) on the states $\mathbf{v}$ and a domain Ω for the parameter values.

Output For each parameter k_i, either returns that it is strongly identifiable, or that the test was inconclusive.

(Step 1) Using `RosenfeldGroebner` with an elimination ranking $\mathbf{v} > \mathbf{y}$, eliminate the variables $\mathbf{v}$, and obtain a set $\mathcal{S} = \{S_1, \ldots, S_\ell\}$ of IO-equations of the input PDE system. We denote the set of their coefficients by $\mathcal{C}$.

(Step 2) For each j, $1 \leqslant j \leqslant \ell$, write S_j in the form

$$F_j = p_{0,j} + \sum_{i=1}^{L_j} a_{i,j} \cdot p_{i,j},$$

with $a_{i,j} \in \mathbb{C}(\mathbf{k})$ and $p_{i,j} \in \mathbb{C}\{\mathbf{y}\}$ (see remark 3). Compute the Wronskians $\mathrm{Wr}_{j,x}$ and $\mathrm{Wr}_{j,t}$ of $p_{1,j}, \ldots, p_{L_j,j}$ with respect to ∂_x and ∂_t, respectively.

(Step 3) For each j, $1 \leqslant j \leqslant \ell$,compute the normal forms $N_{j,x}$ and $N_{j,t}$ of $\mathrm{Wr}_{j,x}$ and $\mathrm{Wr}_{j,t}$, respectively, w.r.t. the input PDE system,and obtain a sufficient condition $\mathcal{I} = \bigwedge_j (N_{j,x} \neq 0 \vee N_{j,t} \neq 0)$ for the identifiability of $\mathcal{C}$.

(Step 4) Check if $\mathcal{I}$ holds under the requirements $\mathcal{R}$ and for the parameters in Ω[10].

(Step 5) If $\mathcal{I}$ does not hold, **return** 'inconclusive' for every parameter.

(Step 6) If $\mathcal{I}$ does hold, **return** 'identifiable' for every parameter k_i such that $k_i \in \mathbb{C}(\mathbf{k})$ (can be checked with, e.g. [27, section 1.3], see [28] for implementation), and 'inconclusive' for the rest of the parameters.

[10] Since there are almost no assumptions on the requirements, this step is non-algorithmic. We show, how to do this in practice in the next section.

5. Examples of PDE identifiability

In this section, we consider several models arising in mathematical biology (section 5.1), as well as other natural phenomena (section 5.2). We use proposition 1 and algorithm 2, to test the strong identifiability of the parameters in these models.

5.1. PDEs arising in mathematical biology

We study four well-known, and increasingly complex, PDE systems in mathematical biology [22]. All of these examples use parabolic PDEs.

Example 11 (Scalar Reaction–Diffusion equation). We start by considering the following reaction–diffusion equation in which c represents the concentration of a diffusible nutrient, such as oxygen or glucose, which is consumed at a rate which is an increasing, saturating function of its concentration [22]:

$$\partial_t c(x,t) = d\partial_x^2 c(x,t) + \frac{\lambda c(x,t)}{c_0 + c(x,t)}, \tag{24}$$

where the set of parameters is $\{d, c_0, \lambda\}$, and the boundary conditions are given by:

$$\partial_x c(x,t)(0,t) = 0 \tag{25}$$

$$c(R,t) = 1 \tag{26}$$

$$c(x,0) = 1, \quad 0 \leqslant x \leqslant R. \tag{27}$$

Following definition 2, our field is $\mathbb{K} = \mathbb{R}$ and $\Omega = \mathbb{R}_+^3$. We follow algorithm 2 to check the strong identifiability of the parameters of (24). Details of the computations can be found in the MAPLE worksheet `nutrient.mpl`[11].

Considering the numerator of the rational function (24), i.e. the differential polynomial

$$-dc(x,t)\partial_x^2 c(x,t) - dc_0\partial_x^2 c(x,t) + c(x,t)\partial_t c(x,t) + c_0\partial_t c(x,t) - \lambda c(x,t), \tag{28}$$

we collect four monomials of (28) whose coefficient (with respect to the elements in $\mathbb{C}(d, c_0, \lambda)$) is not 1, and compute W, the determinant of their Wronskian to check if it is nonsingular. To do so, we compute the normal form of W (using Rosenfeld–Gröbner), and check when its coefficients are zero.

Note that if we obtain nonsingularity of the Wronskian from a subset of the coefficient, it implies that the Wronskian is nonsingular. The first ten coefficients are zero if and only if

$$\partial_t c(x,t) = 0 \quad \text{or} \quad \partial_x c(x,t) = 0. \tag{29}$$

So we investigate the following two cases.

Case 1. $\partial_t c(x,t) = 0$. In this case, the function c does not depend on t anymore, and therefore, $c(x,t) = c(x)$. Using the boundary conditions (26) and (27), we obtain $c(x) = 1$, a constant function. On the other hand, considering $\partial_t c(x,t) = 0$, the differential polynomial (28) will be simplified to the following polynomial (which is the LHS of ODE, rather than the original PDE):

$$-dc(x)\partial_x^2 c(x) - dc_0\partial_x^2 c(x) - \lambda c(x). \tag{30}$$

[11] https://github.com/rahkooy/PDE-Identifiability.

Substituting $c(x) = 1$ into (30), we obtain $-\lambda$, which is not zero, as the parameters are assumed to be positive. So this case cannot happen.
Case 2. $\partial_x c(x,t) = 0$. This condition means that c does not depend on x, hence, $c(x,t) = c(t)$. So substituting this condition into the PDE (24), we obtain the following ODE:

$$\partial_t c(t) = \frac{\lambda c(t)}{c_0 + c(t)}. \tag{31}$$

Using boundary condition (26), i.e. $c(R,t) = 1$, we obtain $\partial_t c(t) = 0$. Therefore ODE (31) is equal to zero if and only if

$$\frac{\lambda c(t)}{c_0 + c(t)} = \frac{\lambda}{c_0 + 1} = 0, \tag{32}$$

which can happen only if $\lambda = 0$. This is impossible according to our assumption on the positivity of the parameters, i.e. $\Omega = \mathbb{R}^3_+$. So Case 2 neither can happen.

In conclusion, none of the cases considered above can happen. This means that the Wronskian matrix is non-singular. So, by proposition 1, the coefficients of the PDE (28), i.e. $\{d, dc_0, c_0, \lambda\}$, are all strongly identifiable.

Example 12 (Fisher's equation). Next, we consider Fisher's equation that describes the diffusive spread of a species which undergoes logistic growth [22]. Fisher's equation is given by the following PDE:

$$\partial_t n(x,t) = d\partial_x^2 n(x,t) + rn(x,t)\left(1 - \frac{n(x,t)}{k}\right), \tag{33}$$

where $n(x,t)$ is the input function, x,t are the variables, and d,r,k are the parameters. The boundary conditions are given by

$$n(x,t) \to \begin{cases} k, & x \to -\infty \\ 0, & x \to \infty, \end{cases} \tag{34}$$

and the initial condition is given by prescribed $u(x,0)$ as follows, which is compatible with the boundary conditions (34).

$$n(x,0) = n_0(x) = \frac{k\mathrm{e}^{-\alpha x}}{1 + \mathrm{e}^{-\alpha x}}. \tag{35}$$

Following definition 2, our field is $\mathbb{K} = \mathbb{R}$ and $\Omega = \mathbb{R}^3_+$. Below we follow algorithm 2 for checking the strong identifiability of the parameters. Details of the computations can be found in the MAPLE worksheet `fisher.mpl`[12]. Simplifying (33), we obtain

$$\partial_t n(x,t) - d\partial_x^2 n(x,t) - rn(x,t) + \frac{rn(x,t)^2}{k}, \tag{36}$$

from which we collect all of the monomials, except for $\partial_t n(x,t)$ whose coefficient is 1, and compute W, the determinant of their Wronskian. Using Rosenfeld–Gröbner, we compute the normal form of the determinant of W, which is a rational function. We would like to check if this rational function is identically zero. Equivalently, we would like to check if the numerator of this rational function, say N, is zero. For this, we consider the coefficients of N as a polynomial in terms of parameters. There are four such coefficients (which are differential polynomials in terms of variables x and t).

[12] https://github.com/rahkooy/PDE-Identifiability.

Computing the coefficients of the normal form of W, one can see that the coefficients are zero if and only if

$$\partial_x n(x,t) = 0 \quad \text{or} \quad \partial_t n(x,t) = 0, \tag{37}$$

which leads to the following cases.

Case 1. $\partial_x n(x,t) = 0$. In this case, the function $n(x,t)$ does not depend on x, hence $n(x,t) = n(t)$. However, the initial condition (35) implies that n is a function of x unless $\alpha = 0$, which cannot happen as the parameters are supposed to be positive.

Case 2. $\partial_t n(x,t) = 0$. This case implies that n does not depend on t, hence, $n(x,t) = n(x)$. From the initial condition (35), we have that

$$n(x) = n_0(x) = \frac{k\mathrm{e}^{-\alpha x}}{1+\mathrm{e}^{-\alpha x}}. \tag{38}$$

We substitute $\partial_t n(x,t) = 0$ into Fisher's equation (33) to obtain the following ODE:

$$-d\partial_x^2 n(x) - rn(x) + \frac{rn(x)^2}{k} = 0. \tag{39}$$

Equation (38) must satisfy ODE (39). Evaluating the ODE at $n(x)$, we obtain

$$\frac{\left(\left(\alpha^2 d - r\right)\mathrm{e}^{-\alpha x} - \alpha^2 d - r\right)k\mathrm{e}^{-\alpha x}}{\left(1+\mathrm{e}^{-\alpha x}\right)^3}. \tag{40}$$

Equation (40) is zero if and only if its numerator is zero, which is the case if and only if either $k = 0$ (which is not possible according to our assumption that parameters are positive), or

$$\left(\alpha^2 d - r\right)\mathrm{e}^{-\alpha x} - \alpha^2 d - r = 0. \tag{41}$$

The above equation can happen only if the coefficient of the exponential term, as well as the constant term are zero. This leads to the equations

$$\alpha^2 d - r = 0 \tag{42}$$

$$-\alpha^2 d - r = 0, \tag{43}$$

which leads to $2\alpha^2 d = 0$. But this cannot happen as α and d are assumed to be non-zero.

So from the above discussions, we conclude that none of the above two cases can happen, hence, the coefficients of the Fisher equation (33), that is, by proposition 1, these functions of parameters are strongly identifiable: d, $\frac{r}{k}$ and $\frac{1}{k}$. By the second part of proposition 1, the parameters d, r, k are strongly identifiable.

Example 13 (Coupled Reaction–Diffusion Equations). Next, we consider the following system of two coupled reaction–diffusion equations. Here species u and v undergo random motion and logistic growth while competing for resources [22]. The PDEs are:

$$\begin{cases} \partial_t u(x,t) = d_1 \partial_x^2 u(x,t) + u(x,t)\left(a_1 - b_1 u(x,t) - c_1 v(x,t)\right), \\ \partial_t v(x,t) = d_2 \partial_x^2 v(x,t) + v(x,t)\left(a_2 - b_2 u(x,t) - c_2 v(x,t)\right), \\ y_1(x,t) = u(x,t), \\ y_2(x,t) = v(x,t). \end{cases} \tag{44}$$

The model parameters are $a_1, b_1, c_1, d_1, a_2, b_2, c_2, d_2$. The boundary conditions are given by

$$u(x,t) \to \begin{cases} \frac{a_1}{b_1} & x \to -\infty \\ 0 & x \to \infty \end{cases} \tag{45}$$

$$v(x,t) \to \begin{cases} \frac{a_2}{b_2} & x \to \infty \\ 0 & x \to -\infty \end{cases} \tag{46}$$

and the initial conditions are given by prescribed $u(x,0)$ and $v(x,0)$, e.g.

$$u(x,0) = u_0(x) = \frac{\left(\frac{a_1}{b_1}\right) \mathrm{e}^{-\alpha_1 x}}{1 + \mathrm{e}^{-\alpha_1 x}} \tag{47}$$

$$v(x,0) = v_0(x) = \frac{\left(\frac{a_2}{b_2}\right) \mathrm{e}^{-\alpha_2 x}}{1 + \mathrm{e}^{-\alpha_2 x}}. \tag{48}$$

We note that for the special case with $a_1 < 0 = b_1 = b_2$ equations (44) reduce to the classical Lotka-Volterra equations with random motion.

Following definition 2, our field is $\mathbb{K} = \mathbb{R}$ and $\Omega = \mathbb{R}^8_+$. Below we follow our method (2) for testing the strong identifiability of the parameters. Details of the computations can be found in the MAPLE worksheet `LV-PDE.mpl`[13].

For the first equation, the normal form of the determinant of the Wronskian yields a polynomial with 34 coefficients. We have considered 22 first coefficients and obtained that the determinant of the Wronskian is zero if and only if

$$\partial_x u(x,t) = 0 \quad \text{or} \quad \partial_t u(x,t) = \partial_t v(x,t) = 0 \quad \text{or} \quad v(x,t) = 0, \tag{49}$$

which leads us to the following cases.

Case 1. $\partial_x u(x,t) = 0$. In this case, the derivatives of $u(x,t)$ with respect to x is zero, which means that the function u does not depend on x, i.e. $u(x,t) = u(t)$. However, according to the initial condition (47), u depends on x, unless $-\alpha_1 = 0$, in which case $u = \frac{a_1}{b_1}$ is a constant function. Using the boundary condition (45) when $x \to -\infty$, functions u becomes zero. This implies that $\frac{a_1}{b_1} = 0$, which cannot happen as we have assumed that the parameters are nonzero. So this case does not happen either.

Case 2. $\partial_t u(x,t) = \partial_t v(x,t) = 0$. In this case, u and v do not depend on it, i.e. $u(x,t) = u(x)$ and $v(x,t) = v(x)$. Since the initial conditions (47) and (48) only depend on x, therefore,

$$u(x,t) = u(x) = \frac{\left(\frac{a_1}{b_1}\right) \mathrm{e}^{-\alpha_1 x}}{1 + \mathrm{e}^{-\alpha_1 x}} \tag{50}$$

$$v(x,t) = v(x) = \frac{\left(\frac{a_2}{b_2}\right) \mathrm{e}^{-\alpha_2 x}}{1 + \mathrm{e}^{-\alpha_2 x}}. \tag{51}$$

On the other hand, substituting $\partial_t u(x,t) = \partial_t v(x,t) = 0$ into the original PDE system (44), one obtains the following two ODEs:

$$-d_1 \partial_x^2 u(x) - u(x)(a_1 - b_1 u(x) - c_1 v(x)) = 0 \tag{52}$$

$$-d_2 \partial_x^2 v(x) - v(x)(a_2 - b_2 u(x) - c_2 v(x)) = 0. \tag{53}$$

[13] https://github.com/rahkooy/PDE-Identifiability.

Therefore, $u(x)$ and $v(x)$ should satisfy the ODEs (52) and (53). Having substituted (50) into the ODEs (52), one obtains

$$\frac{1}{b_1\left(1+\mathrm{e}^{-ax}\right)^3}\left(a_1\mathrm{e}^{-ax}\left(\left(d_1a^2+2c_1v(x)-a_1\right)\mathrm{e}^{-ax}-d_1a^2+v(x)\,\mathrm{e}^{-2ax}c_1+c_1v(x)-a_1\right)\right). \tag{54}$$

Finally, substituting (51) into the above, we obtain a rational function of the form

$$\frac{1}{c_2\left(1+\mathrm{e}^{bx}\right)b_1\left(1+\mathrm{e}^{-ax}\right)^3}F(x)\,a_1\mathrm{e}^{-ax}, \tag{55}$$

where

$$\begin{aligned} F(x) = &-a_2c_1\mathrm{e}^{-x(2a-b)}+\left((-d_1a^2+a_1)c_2-2a_2c_1\right)\mathrm{e}^{x(-a+b)}\\ &-c_2(d_1a^2-a_1)\mathrm{e}^{-ax}+\left(c_2(d_1a^2+a_1)-a_2c_1\right)\mathrm{e}^{bx}\\ &+c_2(d_1a^2+a_1) \end{aligned} \tag{56}$$

The rational function in (55) is identically zero if and only if either $a_1(e)^{-ax}=0$ or $F(x)=0$. Since $a_1\neq 0$, it cannot happen that $a_1(e)^{-ax}=0$. The second case, $F(x)=0$, can happen if the exponential terms appearing in $F(x)$ are linearly dependent, which only can happen if the exponents of those terms are equal. It is enough to consider the cases in which the first exponent is equal to some other exponents. This way, we obtain below four cases, each of which is discussed and it has been shown that none can happen.

For convenience, set

$$u := -a_2c_1, \tag{57}$$

$$w := -d_1a^2+a_1 \tag{58}$$

$$t := d_1a^2+a_1. \tag{59}$$

Then the coefficients of $F(x)$ will be u, wc_2-2u, c_2w, c_2t-u and c_2t. Also, let $y=\mathrm{e}^x$. The four cases are the following.

Case 2.1. $-2a+b=-a+b$. This implies that $a=0$ which cannot happen.
Case 2.2. $-2a+b=-a$. This means that $a=b$, and the exponents become $y^{-a}, y^0, y^{-a}, y^a, y^0$. collecting coefficients of equal exponents, we obtain that

$$u+c_2w=0, \tag{60}$$

$$c_2w-2u+c_2t=0, \tag{61}$$

$$c_2t-u=0. \tag{62}$$

Simplifying the above we have $2u=0$ which is not possible.
Case 2.3. $-2a+b=b$. This case implies that $a=0$ which is not possible.
Case 2.4. $-2a+b=0$. From the conditions of this case, we obtain that $b=2a$, and the exponents will be $y^0, y^a, y^{-a}, y^{2a}, y^0$. since y^a and y^{2a} are linearly independent, if their coefficients do not kill each other, then we are done. This is the case as the coefficients are c_2w-2u and c_2w.

Considering coefficients of the normal form of the determinant of the second Wronskian, we obtain the following conditions:

$$\frac{\partial^2}{\partial_x \partial_t} u(x,t) = \partial_x v(x,t) = 0 \quad \text{or} \tag{63}$$

$$\partial_t u(x,t) = \partial_t v(x,t) = 0 \quad \text{or} \tag{64}$$

$$u(x,t) = 0 \quad \text{or} \tag{65}$$

$$v(x,t) = 0. \tag{66}$$

Three out of the four cases in (63), (64), (65), and (66) have been considered earlier. The only remaining case $\frac{\partial^2}{\partial_x \partial_t} u(x,t) = \partial_x v(x,t) = 0$. Similar to the argument for $\partial_x u(x,t) = 0$, one can check that $\partial_x v(x,t) = 0$ cannot happen. So this case is also impossible.

In conclusion, none of the Wronskians can be identically singular. Hence, by proposition 1, the coefficients of the PDEs (44) are strongly identifiable. Since the coefficients of the system are the parameters, all parameters are strongly identifiable.

Example 14 (Single Output Lotka Volterra). In this example, we consider the single output version of the Coupled Reaction–Diffusion Equations studied in example 13:

$$\begin{cases} \partial_t u(x,t) = d_1 \partial_x^2 u(x,t) + u(x,t)\left(a_1 - b_1 u(x,t) - c_1 v(x,t)\right), \\ \partial_t v(x,t) = d_2 \partial_x^2 v(x,t) + v(x,t)\left(a_2 - b_2 u(x,t) - c_2 v(x,t)\right), \\ y(x,t) = u(x,t). \end{cases} \tag{67}$$

The initial and boundary conditions are the same as the Coupled Reaction–Diffusion Equations and are given by (45), (46), (47), and (48). Similarly, the ground field is $\mathbb{K} = \mathbb{R}$ and $\Omega = \mathbb{R}_+^8$.

For this example, we initially tried to apply algorithm 2. We used [28] applying `FieldToIdeal` and then `FilterGenerators` to regroup the monomials and to simplify the system, and obtained a 13×13 matrix instead of the original 17×17 Wronskian. However, computing the determinant (and then normal form) of this simpler matrix was not possible within a reasonable time and memory. Hence, instead of computing directly the normal form of the determinant of the Wronskian, we used the following steps to make computations faster:

(i) First, we compute the normal form of each entry of the Wronskian
(ii) Secondly, using the equations of the system (67), we eliminate the derivatives of $u(x,t)$ and $v(x,t)$ with respect to t, so that the equations only depend on u, v and their derivatives with respect to x. Then we could substitute the initial conditions efficiently to the system (substituting initial conditions into the original system is very time-consuming).
(iii) Third, we substituted random values for parameters as computations with symbolic parameters were not possible in a reasonable time.
(iv) Lastly, we computed the numeric value of the determinant of the Wronskian, evaluated in a generic point x.

While computing the determinant of the Wronskian and its normal form did not finish within three days, the above optimizations made the computation finish in less than four hours, most of which is spent on normal form computations. Having stored the output of the normal forms, one can carry on the computations for different values of x and the parameters in the initial conditions in just less than a second.

As the determinant was not zero in a generic point, we conclude that the determinant is not a zero function for random nonzero values of the parameters. Although this does not prove strong identifiability, however, we succeeded in presenting strong numeric evidence that generically the parameters are identifiable. Additional studies can check particular values of the parameters that vanish the Wronskian. We note that due to the lack of resources for symbolic computations, we chose random values for parameters. For the details of the computations, we refer to our MAPLE code `LV-Single-Output.mpl`[14] Note that the output of `LV-Single-Output-NormalForm.mp` is used in `LV-Single-Output.mpl`, and to run `LV-Single-Output-NormalForm.mp`, the package `ComputeIdentifiableFunctions.mpl` from [28] is required.

Finally, we also see that the parameters c_1 and c_2 are not identifiable using the following argument. Following definition 2, let

$$\mathbf{k}_1 = (a_1, b_1, c_1, d_1, a_2, b_2, c_2, d_2), \quad \mathbf{v}_1 = (u, v)$$
$$\mathbf{k}_2 = (a_1, b_1, \lambda c_1, d_1, a_2, b_2, \lambda c_2, d_2), \quad \mathbf{v}_2 = (u, v/\lambda),$$

where λ is an arbitrary nonzero number. One sees that, substituting $\mathbf{k}_2$ and $\mathbf{v}_2$ into (67), λ will be eliminated and we will obtain (67) again. However, $\mathbf{k}_1$ and $\mathbf{k}_2$ are not equal. This means that $\mathbf{k}_1$ and $\mathbf{k}_2$ are not identifiable. As $\mathbf{k}_1$ and $\mathbf{k}_2$ only differ in the values of c_1 and c_2, one can conclude that c_1 and c_2 are not identifiable.

Example 15 (A Reaction–Diffusion Model of Cancer Invasion). Our final example from mathematical biology is a PDE model of cancer invasion which couples two reaction–diffusion equations for the concentrations of tumour cells $v(x,t)$ and acid (or pH) $w(x,t)$ with a time-dependent ODE for healthy cells $u(x,t)$. The healthy cells and the cancer cells undergo logistic growth and compete with each other for space. The healthy cells do not move but they are killed by acid which is produced by the tumour cells and undergoes natural decay while it diffuses through the domain. The diffusive movement of the cancer cells is assumed to be a linearly decreasing function of the concentration of healthy cells [23]. The model is given by the following three PDEs:

$$\partial_t u(x,t) = r_1 u(x,t)\left(1 - \frac{u(x,t)}{k_1} - \frac{v(x,t)}{k_2} a_{12}\right) - d_1 w(x,t)\, u(x,t), \tag{68}$$

$$\partial_t v(x,t) = r_2 v(x,t)\left(1 - \frac{v(x,t)}{k_2} - \frac{u(x,t)}{k_1} a_{21}\right) + d_2 \partial_x\left((1 - u(x,t))\,\partial_x v(x,t)\right), \tag{69}$$

$$\partial_t w(x,t) = d_4 \partial_x^2 w(x,t) + r_3 v(x,t) - d_3 w(x,t), \tag{70}$$

along with the output equations

$$y_1(x,t) = u(x,t), \tag{71}$$
$$y_2(x,t) = v(x,t), \tag{72}$$
$$y_3(x,t) = w(x,t). \tag{73}$$

The parameters of the system are $r_1, k_1, a_{12}, k_2, d_1, r_2, a_{21}, d_2, d_3, r_3, d_4$, the boundary conditions are given by

$$u(x,t) \to \begin{cases} k_1, & x \to +\infty \\ 0, & x \to -\infty \end{cases} \tag{74}$$

[14] https://github.com/rahkooy/PDE-Identifiability.

$$v(x,t) \to \begin{cases} 0, & x \to +\infty \\ k_2, & x \to -\infty \end{cases} \tag{75}$$

$$w(x,t) \to \begin{cases} 0, & x \to +\infty \\ \frac{k_2 r_3}{d_3}, & x \to -\infty, \end{cases} \tag{76}$$

and the initial conditions are given by prescribed $u(x,0)$ and $v(x,0)$, e.g.

$$w(x,0) = 0 \tag{77}$$

$$u(x,0) = \frac{k_1 \mathrm{e}^{\gamma_1 x}}{1 + \mathrm{e}^{\gamma_1 x}} \tag{78}$$

$$v(x,0) = \frac{k_2 \mathrm{e}^{-\gamma_2 x}}{1 + \mathrm{e}^{-\gamma_2 x}}. \tag{79}$$

Our ground field is $\mathbb{K} = \mathbb{R}$ and $\Omega = \mathbb{R}^{11}_{+}$, corresponding to the number of parameters.

Details of the computations can be found in the MAPLE worksheet `reaction-diffusion.mpl`[15].

We consider each of the three equations separately, computing three Wronskians and checking if they are nonsingular. We note that for the third equation, as there are no monomials with coefficient 1, we divide the polynomial by $k_1 k_2$ so that it has a monomial with coefficient one. Below is the summary of our computations.

- The first Wronskian yields 40 coefficients. Considering ten of the coefficients, Rosenfeld–Gröbner results in the following conditions:

$$\partial_x u(x,t) = 0 \quad \text{or} \quad v(x,t) = 0. \tag{80}$$

  The above conditions can easily be refuted by looking at the boundary and initial conditions, using arguments similar to the Coupled Reaction–Diffusion equations.
- For the second equation, the normal form contains 8 coefficients. Our procedure results in the following conditions for Wronskian to be singular:

$$w(x,t)\frac{\partial w(x,t)}{\partial t \partial x} = \frac{\partial w(x,t)}{\partial t}\frac{\partial w(x,t)}{\partial x} \quad \text{or} \quad w(x,t) = 0 \quad \text{or} \quad v(x,t) = 0. \tag{81}$$

  The second and third conditions, i.e. $w(x,t) = 0$ and $v(x,t) = 0$ can be easily refuted using boundary and initial conditions. For the first condition, we show that one can solve using the specified initial condition and obtain only zero solution. More precisely, substituting (77) in the first condition, one obtains that either $\frac{\partial w(x,t)}{\partial x} = 0$ at $t = 0$ or $\frac{\partial w(x,t)}{\partial t} = 0$ at $t = 0$. One can easily check that both of these contradict the initial and boundary conditions, as the parameters are not allowed to be zero.
- For the third equation, the first ten coefficients result in the following conditions

$$\frac{\partial u(x,t)}{\partial x} = 0 \quad \text{or} \quad v(x,t) = 0 \tag{82}$$

  The second condition ($v(x,t) = 0$) can be trivially refuted. For the first conditions, adding $\frac{\partial u(x,t)}{\partial x}$ to the system and computing Rosenfeld–Gröbner, we obtain 9 equations, three of

[15] https://github.com/rahkooy/PDE-Identifiability.

which are the input–output equations, three are the partial derivatives of the output equations with respect to x, and the remaining three equations involve the parameters. The latter three are of interest to us. They show that the states are not constant with respect to x. One can check that the boundary and initial conditions would imply that several parameters are zero, which is not permitted according to our assumptions. This can simply be seen as the normal forms of u, v, and w with respect to the Rosenfeld–Gröbner are zero.

Therefore, proposition 1 implies that the coefficients of the system are strongly identifiable. Taking into account the positivity of the parameters, we can conclude that all the parameters are strongly identifiable.

5.2. PDEs from applied mathematics

Finally, in this section, we consider two well-known PDEs in applied mathematics that model natural phenomena.

Example 16. The following PDE is an example of an elliptic PDE.

$$\partial_x^2 u(x,y) + \partial_y^2 u(x,y) = \theta, \tag{83}$$

where $0 \leqslant x \leqslant L$ and $0 \leqslant y \leqslant H$. The boundary conditions are

$$u(x,H) = \frac{\alpha x}{L} \tag{84}$$

$$u(L,y) = \frac{\alpha y}{H}, \tag{85}$$

and the initial conditions are

$$u(x,0) = 0 \tag{86}$$

$$u(0,y) = 0. \tag{87}$$

The parameters of the system are θ and α, and the domain for parameters is $\Omega = \mathbb{R}_+^2$.

In order to remove the parameter α from the boundary condition, one can define a new variable $v := u/\alpha$. Then the new equation and boundary conditions will be

$$\alpha\partial_x^2 v(x,y) + \alpha\partial_y^2 v(x,y) = \theta, \tag{88}$$

the boundary conditions will be

$$v(x,H) = \frac{x}{L} \tag{89}$$

$$v(L,y) = \frac{y}{H}, \tag{90}$$

and the initial conditions will be

$$\alpha v(x,0) = 0 \tag{91}$$

$$\alpha v(0,y) = 0. \tag{92}$$

Since α is assumed to be non-zero, the initial conditions become

$$v(x,0) = 0 \tag{93}$$

$$v(0,y) = 0. \tag{94}$$

Dividing both sides of (88) by α, we obtain $\partial_x^2 v(x,y) + \partial_y^2 v(x,y) = \frac{\theta}{\alpha}$. Hence, $\frac{\theta}{\alpha}$ is strongly identifiable, as it is in terms of derivatives of $v(x,y)$, however, the parameters α and θ are not identifiable. For the special case of $\alpha = 1$, the parameter θ will be strongly identifiable.

Remark 4. Note that the current work does not address the general case of systems with parameters in the boundary conditions. This is a potential future work using prolongations as in SIAN [9].

Example 17. The following PDE is the well-known *wave equation* and is an example of a hyperbolic PDE.

$$\partial_t^2 u(x,t) - \sigma^2 \partial_x^2 u(x,t) = 0, \tag{95}$$

where σ, the parameter, is the wave speed. The initial conditions are given by

$$u(x,0) = L - x, \quad \partial_t u(x,0) = \beta. \tag{96}$$

The output function is $y(x,t) = u(x,t)$. By d'Alembert's formula [35, theorem 2.15], (95) and (96) define a unique solution

$$y(x,t) = -x + \beta t + L. \tag{97}$$

Following definition 2, our ground field is $\mathbb{K} = \mathbb{R}$ and $\Omega = \mathbb{R}_+$. Let us now try to apply algorithm 2 (proposition 1) to see that computing Wronskian is essential. The IO-equation is

$$\partial_t^2 y(x,t) - \sigma^2 \partial_x^2 y(x,t) = 0. \tag{98}$$

Of its two monomials, the coefficient of $\sigma^2 \partial_x^2 y(x,t)$ is not one. The Wronskian of this monomial (with respect to both x and t) is itself. Furthermore, this monomial $\partial_x^2 y(x,t)$ vanishes on every solution (97), so algorithm 2 is not applicable here. Finally, since the solution (97) depends only on the initial conditions and not on σ, σ is nonidentifiable by definition 2.

6. Conclusions

It would be of great practical interest to develop a fully automated software package, e.g. in Maple, Julia, or Python for checking parameter identifiability of PDE models (1). The potential bottlenecks to overcome include the following:

- computationally use the initial and boundary conditions to check that the Wronskian does not vanish,
- automatate the early termination criteria, which we used in our examples, to tame the computational complexity of the differential algebra component of our algorithm to check the vanishing/non-vanishing of the Wronskian.

As another future direction, in order to make our approach more accessible to the PDE community, it is important to address the problem of the existence of solutions of the PDE systems that we consider, similar to the results in [14]. The authors in [14] consider a master–slave model of two species, where the slave one diffuses but the master does not. The master model is the following ODE system

$$\begin{cases} \partial_t \zeta = F(t,\zeta) \\ \zeta(0) = \zeta_0, \end{cases} \tag{99}$$

where $\zeta_0 \in C(\Omega)$ (Ω a bounded domain) and $F : \mathbb{R} \to \mathbb{R}^p \times \mathbb{R}^p$ is piecewise continuous with respect to the first component and uniformly Lipschitz continuous with respect to the second component. The slave model is the following system of reaction–diffusion equations that depend on ζ in the master model

$$\begin{cases} \partial_t U + BU = G(t, \zeta, U) \\ U(0) = U_0, \end{cases} \tag{100}$$

where B is a diagonal operator satisfying certain properties. While it is known that the classical ODE system of the master model has a unique solution, in [14], the authors show that the slave model also admits a unique local solution.

Data availability statement

The data that support the findings of this study are openly available at the following URL/DOI: https://github.com/rahkooy/PDE-Identifiability.

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References

[1] Stumpf M, Balding D J and Girolami M 2011 *Handbook of Statistical Systems Biology* (Wiley)
[2] Marsh L, Dufresne E, Byrne H M and Harrington H A 2022 *Bull. Math. Biol.* **84** 137
[3] Ma M, Huang Z and Ou C 2019 *Nonlinearity* **32** 3143
[4] Simpson M J, Baker R E, Vittadello S T and Maclaren O J 2020 *J. R. Soc. Interface* **17** 20200055
[5] Browning A P, Sharp J A, Murphy R J, Gunasingh G, Lawson B, Burrage K, Haass N K and Simpson M 2021 *eLife* **10** e73020
[6] Hong H, Ovchinnikov A, Pogudin G and Yap C K 2020 *Commun. Pure Appl. Math.* **73** 1831–79
[7] Ritt J F 1950 *Differential Algebra* (Dover Publications Inc.)
[8] Bellu G, Saccomani M P, Audoly S and DAISY D'A L 2007 *Comput. Methods Programs Biomed.* **88** 52–61
[9] Hong H, Ovchinnikov A, Pogudin G and SIAN Y C 2019 *Bioinformatics* **35** 2873–4
[10] Meshkat N, Kuo C and DiStefano J 2014 *PLoS One* **9** e110261
[11] Ilmer I, Ovchinnikov A and Pogudin G 2021 Web-based structural identifiability analyzer *Comput. Methods Syst. Biol.* **12881** 254–65

[12] Dong R, Goodbrake C, Harrington H and Pogudin G 2023 *SIAM J. Appl. Algebra Geom.* **7** 194–235
[13] Bates D, Hauenstein J and Meshkat N 2019 *PLoS One* **14** e0226299
[14] Verdière N, Manceau D, Zhu S and Denis-Vidal L 2020 *Appl. Math. Comput.* **375** 125067
[15] Zhu S and Verdière N 2018 *Ecol. Complex.* **34** 80–88
[16] Renardy M, Kirschner D and Eisenberg M 2022 *J. Math. Biol.* **84** 9
[17] Ciocanel M V, Ding L, Mastromatteo L, Reichheld S, Cabral S, Mowry K and Sandstede B 2024 *Bull. Math. Biol.* **86** 36
[18] Browning A P, Tască M, Falcó C and Baker R E 2024 *Proc. R. Soc.* A **480** 20230911
[19] Saccomani M, Audoly S and D'Angiò L 2003 *Automatica* **39** 619–32
[20] Gerbet D and Röbenack K 2021 *Algorithms* **14** 255
[21] Boulier F, Lazard D, Ollivier F and Petitot M 2009 *Appl. Algebra Eng. Commun. Comput.* **20** 73–121
[22] Murray J D 2013 *Mathematical Biology: I. An Introduction* (Springer)
[23] Gatenby R A and Gawlinski E T A 1996 *Cancer Res.* **56** 5745–53
[24] Anstett-Collin F, Denis-Vidal L and Millérioux G A 2020 *Annu. Rev. Control* **50** 139–49
[25] Ovchinnikov A, Pogudin G and Thompson P 2021 *Appl. Algebra Eng., Commun. Comput.* **34** 165–82
[26] Boulier F and Lemaire F 2000 Computing canonical representatives of regular differential ideals *Proc. 2000 Int. Symp. on Symbolic and Algebraic Computation (ISSAC) (ACM)* pp 38–47
[27] Müller-Quade J and Steinwandt R 1999 *J. Symb. Comput.* **27** 143–70
[28] 2023 Allidentifiablefunctions (https://github.com/pogudingleb/Allidentifiablefunctions)
[29] Ovchinnikov A, Pillay A, Pogudin G and Scanlon T 2021 *Syst. Control Lett.* **157** 105030
[30] Kaplansky I 1957 *An Introduction to Differential Algebra* (Hermann)
[31] Milne J S 2020 *Fields and Galois Theory (v4.61)*
[32] Hubert E 2003 Notes on triangular sets and triangulation-decomposition algorithms II: Differential Systems *Proc. 2nd Int. Conf. on Symbolic and Numerical Scientific Computation SNSC'01* (Springer) pp 40–87
[33] Bouziane D, Kandri Rody A and Maârouf H 2001 *J. Symb. Comput.* **31** 631–49
[34] Meshkat N, Eisenberg M and DiStefano J J A algorithm 2009 *Math. Biosci.* **222** 61–72
[35] Olver P 2014 *Introduction to Partial Differential Equations* (Springer)