

# THE UNIQUENESS PROBLEM OF PHYSICAL LAW LEARNING

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## ABSTRACT

Physical law learning is the ambiguous attempt at automating the derivation of governing equations with the use of machine learning techniques. This paper shall serve as a first step to build a comprehensive theoretical framework for learning physical laws, aiming to provide reliability to according algorithms. One key problem consists in the fact that the governing equations might not be uniquely determined by the given data. We will study this problem in the common situation that a physical law is described by an ordinary or partial differential equation. For various different classes of differential equations, we provide both necessary and sufficient conditions for a function from a given function class to uniquely determine the differential equation which is governing the phenomenon. We then use our results to determine in extensive numerical experiments whether a function solves a differential equation uniquely.

**Index Terms**— physical law learning, learning differential equations, machine learning

**This conference paper displays the most important results from the longer version [1], the proofs can also be found in [1].**

## 1. INTRODUCTION

For most of human history, engineers had to derive physical laws by hand. As the usage of data in physics is growing and artificial intelligence is becoming more powerful, engineers and physicists are aiming to apply machine learning to infer the governing laws from experimental data. This has the potential to advance our modeling and understanding of complex dynamics across disciplines. In [2, 3, 4] the possibilities are shown to accurately compute dynamics used in mechanics, biology, environmental science, fluid dynamics,

high-energy physics, electronic science, atomic physics and robotics.

The common assumption is that the underlying physical law is given by a function, an ordinary differential equation (ODE), or a partial differential equation (PDE). In this paper we concentrate on methods, which take data from a solution  $(u(t_i, x_j))_{ij} \subset \mathbb{R}$  of some PDE as input and output the corresponding differential equation. The theory for ODEs can be found in [1].

Contrary to most of the literature to date [2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14], which concentrates solely on methods, we intend to build the foundation to analyze physical law learning from a theoretical point of view in this paper. For this, we focus on the well-definedness of the PDE learning problem: A learning algorithm should for the input  $u$  and some  $n \in \mathbb{N} \setminus \{0\}$  return the function  $F$  describing the unique PDE such that

$$F(u_{\alpha^1}, u_{\alpha^2}, \dots) = \frac{\partial^n u}{\partial t} \quad (1)$$

holds, where  $\alpha^1, \alpha^2, \dots$  are multi-indices. Hence, the learning algorithm aims to approximate the operator  $O$  which maps a solution  $u$  to its corresponding PDE described by the function  $F$ , i.e.,  $O(u) = F$ . This operator  $O$ , however, is only well-defined if for all  $u$  there exists exactly one function  $F$  describing a PDE which is solved by  $u$ . In this paper we assume that there exists at least one function  $F$  such that (1) holds and focus exclusively on the uniqueness of  $F$ .

The non-uniqueness of PDEs is a potential danger for any scientific insights inferred using the existing methods, since an algorithm cannot know which of the possible PDEs to choose. To establish that the uniqueness is indeed not given in general but is highly desirable, we provide the following example, see [8].

**Example 1** *The Korteweg–De Vries (KdV) equation is defined as*

$$u_t = 6uu_x - u_{xxx} \quad (2)$$

*and is solved by the function  $u(t, x) = c/2 \operatorname{sech}^2(\sqrt{c}/2(x - ct - a))$ , where  $\operatorname{sech}(x) = \frac{1}{\cosh(x)}$  is the hyperbolic secant.*

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However,  $u$  also solves the one-way wave equation  $u_t = -cu_x$ . In a situation like this, the learning algorithm cannot know which PDE it has to output and may end up choosing the wrong one [8].

To the best of our knowledge, Example 1 in [8] is the only time this uniqueness problem is mentioned in the physical law learning literature and, furthermore, it is never tackled theoretically.

In this paper we want to raise the awareness of the uniqueness problem, as it is vital when conducting physical law learning to keep in mind what could have gone wrong and to build the foundations for further theoretical investigations of the problem. To achieve that, we provide necessary and sufficient conditions for the uniqueness of PDEs in Section 2. Afterwards in Section 3, we show in extensive numerical experiments that our theory can be used in practice to assess the uniqueness of PDEs.

## 2. UNIQUENESS OF PDES

In this section, we aim to derive conditions which guarantee uniqueness/non-uniqueness of PDEs in the form of (1) for  $u : U \rightarrow \mathbb{R}, U \subset \mathbb{R}^{m+1}$  open.

A first restriction we make is to fix the set of derivatives  $u_{\alpha^1}, \dots, u_{\alpha^k}$  which are allowed to be used, where  $\alpha^1, \dots, \alpha^k \in \mathbb{N}^m$  are some multi-indices. This means that we aim to prove that there exists a unique  $F$  such that  $F(u_{\alpha^1}, \dots, u_{\alpha^k}) = \frac{\partial^n u}{\partial t^n}$  holds. This, however, does not imply uniqueness for a different set of derivatives  $u_{\beta^1}, \dots, u_{\beta^l}$ , i.e., there might be  $G(u_{\beta^1}, \dots, u_{\beta^l}) = \frac{\partial^n u}{\partial t^n}$  with  $G \neq F$ .

We extend this to also allow  $F$  to explicitly depend on  $t$  or  $x$ . For this we denote throughout this paper with the functions  $g_1, \dots, g_k : U \rightarrow \mathbb{R}$  either a projection on a single coordinate, e.g.,  $g_i(t, x) = x_l$ , for some  $l \in \{1, \dots, m\}$ , or any derivative of  $u$  that exists. Thus, we are interested in conditions on  $g_1, \dots, g_k$  and  $\frac{\partial^n u}{\partial t^n}$  such that there exists a unique  $F : \mathbb{R}^k \rightarrow \mathbb{R}$  with  $F(g_1, \dots, g_k) = \frac{\partial^n u}{\partial t^n}$ .

A second restriction we enforce is that we ask for uniqueness of the PDE described by  $F$  in a specific function class. We start in Subsection 2.1 with linear PDEs and go then from polynomial and algebraic PDEs in 2.2 to analytic PDEs in 2.3. Before we show results for specific classes of PDEs we start with one which holds for an arbitrary PDE class and will serve as a foundation for all further results [1].

**Proposition 1** *Let  $n \in \mathbb{N} \setminus \{0\}$  and  $u : U \rightarrow \mathbb{R}, U \subset \mathbb{R}^{m+1}$  open, such that  $\frac{\partial^n u}{\partial t^n}$  exists. Define the mapping  $g = (g_1, \dots, g_k) : U \rightarrow \mathbb{R}^k$ . Let  $V$  be any class of functions mapping from  $\mathbb{R}^k$  to  $\mathbb{R}$  which is closed under addition/subtraction. Assume there exists  $F \in V$  such that  $F(g) = \frac{\partial^n u}{\partial t^n}$ . Then,  $F$  is the only function in  $V$  such that  $F(g) = \frac{\partial^n u}{\partial t^n}$  if and only if there does not exist some  $H \in V \setminus \{0\}$  such that  $H(g) = 0$ .*

This section presents and summarizes the most important results from Section II in [1], omitting the proofs and a more in depth analysis.

### 2.1. Linear PDEs

The smallest set of PDEs we investigate is the class of linear PDEs, which is well understood theoretically and covers important equations such as the heat and wave equation. For this function class there exists an easy condition for uniqueness of the PDE, which is also straightforward to test numerically [1].

**Theorem 1 (Uniqueness for linear PDEs)** *Let  $n \in \mathbb{N} \setminus \{0\}$  and  $u : U \rightarrow \mathbb{R}, U \subset \mathbb{R}^{m+1}$  open, such that  $\frac{\partial^n u}{\partial t^n}$  exists. Define the function  $g = (g_1, \dots, g_k) : U \rightarrow \mathbb{R}^k$ . Assume there exists at least one linear function  $F : \mathbb{R}^k \rightarrow \mathbb{R}$  with  $F(g) = \frac{\partial^n u}{\partial t^n}$ . Then,  $F : \mathbb{R}^k \rightarrow \mathbb{R}$  is the unique linear function with  $F(g) = \frac{\partial^n u}{\partial t^n}$  if and only if  $g_1, \dots, g_k$  are linear independent.*

### 2.2. Polynomial and Algebraic PDEs

The next larger class are polynomial PDEs. It was proven in [1] that the conditions for uniqueness of polynomial PDEs coincide with those for algebraic PDEs. Thus, all the results in this section apply to both classes. Note, that we call a PDE  $\frac{\partial^n u}{\partial t^n} = F(g_1, \dots, g_k)$  algebraic if  $F$  is an algebraic function, i.e., there is a nonzero, irreducible polynomial  $p$  such that  $p(x, F(x)) = 0$ .

Interestingly, uniqueness of polynomial/algebraic PDEs can be described in algebraic [15, 16] terms [1].

**Proposition 2** *Let  $n \in \mathbb{N} \setminus \{0\}$  and  $u : U \rightarrow \mathbb{R}, U \subset \mathbb{R}^{m+1}$  open, such that  $\frac{\partial^n u}{\partial t^n}$  exists. Define  $g = (g_1, \dots, g_k) : U \rightarrow \mathbb{R}^k$  and  $\mathcal{D} = g(U)$ . Assume there is at least one polynomial/algebraic function  $F : \mathbb{R}^k \rightarrow \mathbb{R}$  with  $F(g) = \frac{\partial^n u}{\partial t^n}$ . Then,  $F : \mathbb{R}^k \rightarrow \mathbb{R}$  is the unique polynomial/algebraic function with  $F(g) = \frac{\partial^n u}{\partial t^n}$  if and only if one of the following statements holds:*

- 1) *There exists no algebraic set  $X \neq \mathbb{R}^k$  such that  $\mathcal{D} \subset X$ , where  $\mathcal{D}$  is the image of  $g = (g_1, \dots, g_k)$ .*
- 2) *The correspondence  $I$  of  $\mathcal{D}$  is trivial, i.e.,  $I(\mathcal{D}) = \{0\}$ .*
- 3) *The functions  $g_1, \dots, g_k : U \rightarrow \mathbb{R}$  are algebraically independent over  $\mathbb{R}$ .*

For general functions  $u$  we develop additional sufficient conditions for uniqueness in the next subsection for analytic PDEs, which can also be used for the smaller class of polynomial PDEs and, thus, also for algebraic PDEs. If we restrict  $u$  to algebraic functions, there are further results for polynomial and algebraic PDEs.

The next result shows that there exist at most  $m$  algebraically independent algebraic functions for  $m$  unknowns [17, 1].

**Theorem 2** *Let  $f_1, \dots, f_{m+1} : U \rightarrow \mathbb{R}, U \subset \mathbb{R}^m$  open, be  $m+1$  algebraic functions in  $m$  variables. Then,  $f_1, \dots, f_{m+1}$  are algebraically dependent.*

Since the derivative of an algebraic function is algebraic, if it exists [1], Theorem 2 shows that if  $u$  is an algebraic function, we have to limit the number of derivatives we use, as otherwise it is certain that there are multiple polynomial/algebraic PDEs solved by  $u$ . In the case that we have at least as many unknown variables as functions, it is possible to use the Jacobi criterion [17, 1].

**Theorem 3 (Jacobi criterion for algebraic independence)**

Let  $n \in \mathbb{N} \setminus \{0\}$  and  $u : U \rightarrow \mathbb{R}$ ,  $U \subset \mathbb{R}^{m+1}$  open, an algebraic function such that  $\frac{\partial^n u}{\partial t^n}$  exists. Define  $g = (g_1, \dots, g_k) : U \rightarrow \mathbb{R}^k$  and assume that  $k \leq m + 1$ . Then,  $g_1, \dots, g_k$  are algebraically independent over  $\mathbb{R}$  if and only if there is one point  $(t, x) \in U$  with  $\text{rank}(J_g(t, x)) = k$ .

Theorem 3 is seemingly similar to Theorem 4. However, it shows that for algebraic functions,  $\text{rank}(J_g(t, x)) = k$  is an equivalent condition to uniqueness of polynomial and algebraic PDEs. Theorem 4, on the other hand, holds for arbitrary functions  $u$ , but only gives a sufficient condition for the uniqueness.

### 2.3. Analytic PDEs

The logical extension of polynomials are analytic functions [18], which are functions which can be approximated locally by their Taylor series. The following condition implies the uniqueness of analytic PDEs [1]. As mentioned before, it is only a necessary and not a sufficient condition for uniqueness.

**Proposition 3 (Measure criterion for analytic functions)**

Let  $n \in \mathbb{N} \setminus \{0\}$  and  $u : U \rightarrow \mathbb{R}$ ,  $U \subset \mathbb{R}^{m+1}$  open, such that  $\frac{\partial^n u}{\partial t^n}$  exists. Define  $g = (g_1, \dots, g_k) : U \rightarrow \mathbb{R}^k$  and  $\mathcal{D} = g(U)$ . Assume there is at least one analytic function  $F : \mathbb{R}^k \rightarrow \mathbb{R}$  with  $F(g) = \frac{\partial^n u}{\partial t^n}$ . If  $\lambda^k(\mathcal{D}) > 0$ , then  $F$  is the unique analytic function such that  $F(g) = \frac{\partial^n u}{\partial t^n}$  holds.

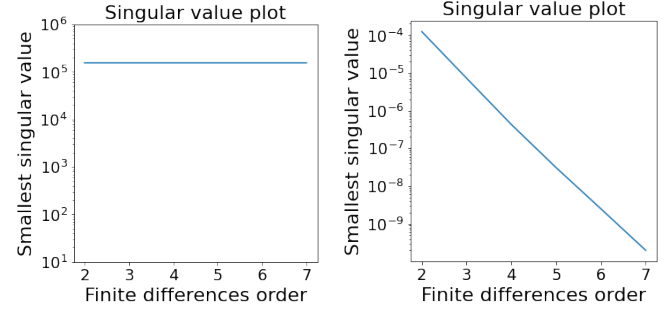
Proposition 3 shows uniqueness in the situation of analytic PDEs, provided that the image of  $g$  is a set with positive measure. The image of a differentiable function, which maps from a lower-dimensional to a higher-dimensional space, is always a null set [19]. Therefore,  $\lambda^k(\mathcal{D}) > 0$  can only be true if  $m + 1 \geq k$ . In this case, the uniqueness of the PDE can also be assessed by investigating the Jacobi matrix of  $g$ .

**Theorem 4 (Jacobi criterion for analytic functions)**

Let  $n \in \mathbb{N} \setminus \{0\}$  and  $u : U \rightarrow \mathbb{R}$ ,  $U \subset \mathbb{R}^{m+1}$  open, such that  $\frac{\partial^n u}{\partial t^n}$  exists. Define  $g = (g_1, \dots, g_k) : U \rightarrow \mathbb{R}^k$ . Assume there is at least one analytic function  $F$  with  $F(g) = \frac{\partial^n u}{\partial t^n}$ . If there exists one point  $(t, x) \in U$  with  $\text{rank}(J_g(t, x)) = k$ , then  $F$  is the unique analytic function such that  $F(g) = \frac{\partial^n u}{\partial t^n}$  holds.

## 3. NUMERICAL EXPERIMENTS

In this section we consider different functions and utilize the theory developed in the last sections to determine whether



(a) Feature matrix  $U = (u(t_i, x_j)_{i,j}, u_x(t_i, x_j)_{i,j})$  for  $u(t, x) = (x + bt) \exp(at)$ .  
(b) Feature matrix  $U$  consisting out of all monomials up to degree 2 of  $u, u_x, u_{xx}$  and  $u_{xxx}$  for  $u(t, x) = \frac{c}{2} \text{sech}^2(\frac{\sqrt{c}}{2}(x - ct - a))$ .

**Fig. 1:** Plot of the lowest singular value of the feature matrix  $U$  using finite differences of different orders.

they solve a PDE uniquely or not. The code of our experiments and additional ones included in [1] is publicly available on github.<sup>1</sup>

### 3.1. Linear PDEs

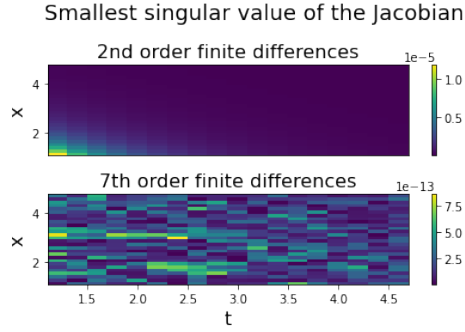
We start again with linear PDEs. We consider the PDE  $u_t = au + bu_x$ , with  $a, b \neq 0$ ,  $u(0, x) = x$ , which is solved by  $u(t, x) = (x + bt) \exp(at)$ . The question we aim to answer in this section is whether there exists a different linear PDE  $u_t = F(u, u_x)$  which is solved by  $u$ . As  $u(t, x) = (x + bt) \exp(at)$  and  $u_x(t, x) = \exp(at)$  are linearly independent, Theorem 1 yields that  $u_t = au + bu_x$  is the unique linear PDE in the form  $u_t = F(u, u_x)$  solved by  $u$ .

Numerically we assess the uniqueness, i.e., the linear dependence of  $u$  and  $u_x$  by computing the least singular value of the matrix  $U = (u(t_i, x_j)_{i,j}, u_x(t_i, x_j)_{i,j})$ . Since computing derivatives numerically is unstable [20], we compute the derivatives for increasing orders of finite differences and check whether the least singular values of these matrices then converge exponentially to 0. This is expected to happen if the true matrix is not full rank since higher order finite differences method have higher order residual terms [20]. The least singular values of  $U$  computed by different finite differences order are displayed in Fig. 1a. As Fig. 1a shows no exponential decay we conclude that the PDE  $u_t = au + bu_x$  is the unique linear PDE in the form  $u_t = F(u, u_x)$  solved by  $u$ .

### 3.2. Polynomial and Algebraic PDEs

For the experiments with polynomial PDEs, we start by revisiting the Korteweg de Vries equation in Section 3.2.1 and consider afterwards the algebraic function  $u(t, x) = 1/(t+x)$  in Section 3.2.2.

<sup>1</sup><https://github.com/Philipp238/physical-law-learning-uniqueness>



**Fig. 2:** Smallest singular value of the Jacobian at different points  $(t_i, x_j)$  of  $g = (u, u_x)$  for  $u(t, x) = 1/(x+t)$ . For the upper image, the derivatives were computed using 2nd order finite differences and, for the lower image, 7th order finite differences were used.

### 3.2.1. Korteweg de Vries equation

We consider Example 1 in this section again and aim to show the ambiguity of  $u_t = F(u, u_x, u_{xx}, u_{xxx})$  for polynomial functions  $F$  numerically.

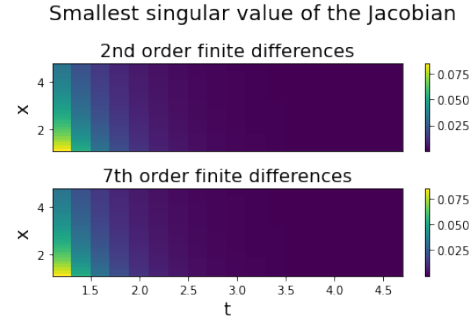
Since  $u$  is not algebraic, we cannot use Theorem 2 and 3. As there are more functions than variables involved, Theorem 4 will not be helpful either as the rank of the Jacobian will be at most  $m + 1 = 2 < 4 = k$ .

Thus, we rely on Proposition 1 and directly search for a nonzero polynomial function  $H$  with  $H(u, u_x, u_{xx}, u_{xxx}) = 0$ . For this we construct a library of monomials of the derivatives and check them for linear independence. We start with monomials up to order 2, i.e., we construct the feature matrix  $U = (u \ u_x \ u_{xx} \ u_{xxx} \ u^2 \ uu_x \ \dots \ u_{xxx}^2)$ . If  $U$  is not full rank, we know that there is a polynomial  $H$  with  $H(u, u_x, u_{xx}, u_{xxx}) = 0$  and, thus, the PDE is not unique by Proposition 1.

The rank of  $U$  can be assessed again by computing the least singular value of  $U$  for increasing finite differences order. This is shown in Fig. 1b. We clearly see that  $U$  is indeed not full rank which means that there exists a polynomial  $p$  of degree 2 such that  $p(u, u_x, u_{xx}, u_{xxx}) = 0$  and, therefore, the KdV equation is not the unique polynomial PDE solved by  $u$ .

### 3.2.2. Algebraic solution

Next we consider the algebraic function  $u(t, x) = 1/(t+x)$  which solves the linear PDE  $u_t = u_x$  and the polynomial PDE  $u_t = -u^2$ . Here, we assume that we know that  $u$  is an algebraic function and we aim to show non-uniqueness of polynomial PDEs of the form  $u_t = F(u, u_x)$  by applying the Jacobi criterion. Fig. 2 shows the smallest singular value of the Jacobian at different data points  $(t_i, x_j)$ . The upper image was created by computing the derivatives using 2<sup>nd</sup> order finite differences and the lower image using 7<sup>th</sup> order finite differences. We see a clear trend from singular values



**Fig. 3:** Smallest singular value of the Jacobian at different points  $(t_i, x_j)$  of  $u(t, x) = (x+t) \arccos(\text{sech}(-t))$ . For the upper image, the derivatives were computed using 2nd order finite differences and, for the lower image, 7th order finite differences were used.

around  $10^{-5}$  to  $10^{-13}$  and, thus, deduce that the Jacobian is at no point  $(t_i, x_j)$  full rank. As  $u$  is algebraic, Theorem 3 yields that  $u$  solves multiple polynomial PDEs.

### 3.3. Analytic PDEs

In this last section we investigate the usefulness of the Jacobi criterion for analytic PDEs. Consider the PDE  $u_t = u_x - \frac{u}{u_x} \sin(u_x)$ . This PDE is solved by  $u(t, x) = (x+t)v(t)$ , for  $t > 0$ , where  $v(t) = \arcsin(\text{sech}(t))$ . The question is if it is the unique analytic PDE of the form  $u_t = F(u, u_x)$  which is solved by  $u$ . Thus, we apply the Jacobian criterion for analytic functions and check the singular values in Fig. 3. As we see no trend towards 0 for the least singular values, we deduce that  $u_t = u_x - \frac{u}{u_x} \sin(u_x)$  is the unique analytic PDE solved by  $u$ .

## 4. CONCLUSION

Even though the non-uniqueness of PDEs is a vital issue for physical law learning applications, it has never been addressed in the literature—to the best of our knowledge—, apart from [8]. To develop a theoretical understanding of the problem, we provide sufficient and necessary conditions for the uniqueness of PDEs in this paper. Furthermore, we deduced algorithms using those conditions to determine numerically if a function solves a unique PDE.

With this paper we built the foundation for theoretical research about physical law learning, a field which has so far only been driven by practical applications. In future work we intend to also add existence results to build a proper base for any theoretical study of physical law learning, like its robustness and computability.

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