Algebraic Identifiability of Partial Differential Equation Models

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Differential Equation Models

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- A **Dynamical system/ODE model** is a system of the form:

$$\Sigma := \begin{cases} \mathbf{x}' = \mathbf{f}(\mathbf{x}, \boldsymbol{\lambda}, \mathbf{u}) \\ \mathbf{y} = \mathbf{g}(\mathbf{x}, \boldsymbol{\lambda}, \mathbf{u}) \\ \mathbf{x}(0) = \mathbf{x}^*, \end{cases}$$

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  - $\mathbf{x}$: state variables
  - $\mathbf{y}$: output variables,
  - $\mathbf{u}$: input variables,
  - $\boldsymbol{\lambda}$: parameters,
  - $\mathbf{x}(0)$: initial conditions,
  - $\mathbf{f}$ and $\mathbf{g}$ are rational function.

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  - $\mathbf{f}$ and $\mathbf{g}$ are rational function.
- We assume $\mathbf{y}(0), \mathbf{y}'(0), \mathbf{y}''(0), \ldots$ can be measured and that $\mathbf{u}$ is also specified/known.

Parameter Identifiability Problem

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- **locally identifiable**: finitely many values for parameters
- **unidentifiable**: infinitely many values for parameters

Example

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- So

$$\lambda_1^2 = \frac{y - \lambda_2}{t},$$

hence, λ_1 locally identifiable.

Existing Approaches

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- Differential Algebra: Take derivatives of the system

$$\Sigma^m := \begin{cases} \mathbf{x}' = \mathbf{f}(\mathbf{x}, \boldsymbol{\lambda}, \mathbf{u}) \\ \vdots \\ \mathbf{x}^{(m)} = \mathbf{f}^{(m)}(\mathbf{x}, \boldsymbol{\lambda}, \mathbf{u}) \\ \mathbf{y}(0) = \mathbf{g}(\mathbf{x}(0), \boldsymbol{\lambda}, \mathbf{u}(0)) \\ \mathbf{y}'(0) = \mathbf{g}'(\mathbf{x}(0), \boldsymbol{\lambda}, \mathbf{u}(0) \\ \vdots \\ \mathbf{y}^{(m)}(0) = \mathbf{g}^{(m)}(\mathbf{x}(0), \boldsymbol{\lambda}, \mathbf{u}(0)) \\ \mathbf{x}(0) = \mathbf{x}^*. \end{cases}$$

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- *"Make"* Σ^m into a polynomial system and use computational algebra techniques, e.g., Gröbner Bases/Rosenfeld-Gröbner.

- Plug in random values of $\hat{\boldsymbol{\lambda}}$ to $\boldsymbol{\lambda}$ and solve the ODE system Σ for the values $\mathbf{y}(0), \mathbf{y}(0)', \mathbf{y}''(0), \ldots, \mathbf{y}^{(m)}(0)$

A Probabilistic Algorithm for ODE Identifiability (SIAN)

- Plug in random values of $\hat{\boldsymbol{\lambda}}$ to $\boldsymbol{\lambda}$ and solve the ODE system Σ for the values $\mathbf{y}(0), \mathbf{y}(0)', \mathbf{y}''(0), \ldots, \mathbf{y}^{(m)}(0)$
- To check if λ_i is globally identifiable we can check whether

$$\lambda_i - \hat{\lambda}_i \in GB(\Sigma^m),$$

  where $GB(\Sigma^b)$ is a Gröbner basis (and the membership can be checked via reduction).

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- Generalisation to a PDE system:

$$\Sigma := \begin{cases} \partial_t \mathbf{x} = \mathbf{f}(\mathbf{x}, \boldsymbol{\lambda}, \mathbf{u}, \partial_t^i \partial_\xi^j \mathbf{x}), \;\; i + j \leq m \\ \mathbf{y} = \mathbf{g}(\mathbf{x}, \boldsymbol{\lambda}, \mathbf{u}) \\ \mathbf{x}(0) = \mathbf{x}^* \\ \text{Boundary Conditions} \end{cases}$$

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- In practice, boundary conditions can be non-algebraic, which can make theory/computations hard.

Algebraic Definition of PDE Identifiability

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- Differential ring:

$$R = \mathbb{C}(\boldsymbol{\lambda})[\partial_t^i \partial_\xi^j \mathbf{x}, \partial_t^i \partial_\xi^j \mathbf{y}, \partial_t^i \partial_\xi^j \mathbf{u} \mid i, j \geq 0]$$

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- Differential ideal associated to the model Σ:

$$I = \langle \partial_t^i \partial_\xi^j (\partial_t \mathbf{x} - \mathbf{f}), \partial_t^i \partial_\xi^j (\mathbf{y} - \mathbf{g}) \mid i, j \geq 0 \rangle \subseteq R$$

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Definition

Let $\hat{\mathbf{x}}, \hat{\mathbf{y}}, \hat{\mathbf{u}}$ be the image of $\mathbf{x}, \mathbf{y}, \mathbf{u}$ in R/I. A parameter $\lambda \in \boldsymbol{\lambda}$ (or a rational function of parameters) is identifiable if

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Theorem

*Let $I \subseteq R$ be the differential ideal corresponding to a PDE model, with **characteristic set** S. A parameter λ in S is identifiable if the polynomials in S, considered as polynomials in variable $\boldsymbol{\lambda}$ with monomial coefficients in R, have linearly independent coefficients.*

Testing PDE Identifiability

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- One can check the linear independence of the monomial coefficients by checking non-singularity of certain Wronskians.

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8. Obtain a sufficient condition $\mathcal{C}$ for normal forms not to be zero
9. Using initial/boundary conditions check if $\mathcal{C}$ holds.

Case Study: Nutrient Reaction–Diffusion

$$-d\frac{\partial c(x,t)}{\partial x^2}c(x,t) - dc_0\frac{\partial c(x,t)}{\partial x^2} + \frac{\partial c(x,t)}{\partial t}c(x,t) + c_0\frac{\partial c(x,t)}{\partial t} - \lambda c(x,t),$$

- Initial Conditions:

$$c(R,t) = 1, \quad c(x,0) = 1, 0 \leq x \leq R$$

- Boundary Conditions:

$$\frac{\partial c(0,t)}{\partial t} = 0.$$

Case Study: Nutrient Reaction–Diffusion

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```
> restart:
```

Setting up the PDE:

```
> eq := diff(c(x,t),t)-d*diff(c(x,t),x$2)-lambda*c(x,t)/(c_0+c(x,t));
```

$$eq := \frac{\partial}{\partial t} c(x,t) - d\left(\frac{\partial^2}{\partial x^2} c(x,t)\right) - \frac{\lambda\, c(x,t)}{c\_0 + c(x,t)}$$ (

Clearing out the numerators. This is our input-output equation (called IO-equation below):

```
> numer(eq);
```

$$-d\left(\frac{\partial^2}{\partial x^2} c(x,t)\right) c(x,t) - d\left(\frac{\partial^2}{\partial x^2} c(x,t)\right) c\_0 + \left(\frac{\partial}{\partial t} c(x,t)\right) c(x,t) + \left(\frac{\partial}{\partial t} c(x,t)\right) c\_0 - \lambda\, c(x,t)$$ (

Creating variables for the monomials of the input-output equation

```
> M1 := simplify(diff(c(x, t), x, x)*c(x, t)):
  M2 := simplify(diff(c(x, t), x, x)):
  M3 := simplify(diff(c(x, t), t)):
  M4 := c(x,t):
```

Case Study: Nutrient Reaction–Diffusion

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Creating the Wronskian of the monomials

```
> with(VectorCalculus):with(LinearAlgebra):
  Wr := simplify(Determinant(Wronskian([M1,M2,M3,M4],x))):
```

Setting up differential algebra to study the Wronskian

```
> with(DifferentialAlgebra):
  R := DifferentialRing(blocks = [c], derivations = [x,t], arbitrary =
  [lambda, c_0, d]):
  RG := RosenfeldGroebner([eq], R):
```

Does the Wronskian vanish? Let us find out by computing the remainder modulo the IO-equation and listing the coefficients of the result as a polynomial in the parameters

```
> cf := coeffs(expand(numer(simplify(NormalForm(Wr, RG)))[1]),[lambda, c_0,
  d]):
> for i from 1 to nops([cf]) do print(cf[i]); print(\n) od;
```

$$3\left(\frac{\partial}{\partial t}c(x,t)\right)^2\left(\frac{\partial^2}{\partial t\partial x}c(x,t)\right)^2c(x,t)^6-3\left(\frac{\partial}{\partial x}c(x,t)\right)^2\left(\frac{\partial^2}{\partial t^2}c(x,t)\right)^2c(x,t)^6$$

Case Study: Nutrient Reaction–Diffusion

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$$-6\left(\frac{\partial}{\partial t}c(x,t)\right)\left(\frac{\partial^2}{\partial t \partial x}c(x,t)\right)^2 c(x,t)^6$$

$$3\left(\frac{\partial^2}{\partial t \partial x}c(x,t)\right)^2 c(x,t)^6$$

(3)

Let us try to get useful consequences of the vanishing of the coefficients (we chose just 10 of those to run the computation faster).

```
> Equations(RosenfeldGroebner([cf[-1],cf[1..10]],R));
```

$$\left[\left[\frac{\partial}{\partial t}c(x,t)\right],\left[\frac{\partial}{\partial x}c(x,t)\right]\right]$$

(4)

- plugging in each of the above into the PDE, we obtain ODEs, and then using the initial conditions one can prove that the above expressions cannot be zero.

Case Study: Fisher's Equation

$$
\Sigma := \begin{cases}
\frac{\partial n(x,t)}{\partial t} - d\frac{\partial n(x,t)}{\partial x^2} - rn(x,t)(1 - \frac{n(x,t)1}{k}), \begin{cases} -\infty < x < \infty \\ 0 < t \end{cases} \\
\text{Boundary Cond:} \quad n(x,t) \to \begin{cases} k & x \to -\infty \\ 0 & x \to +\infty \end{cases} \\
\text{Initial Conds:} \quad n(x,0) = n_0(x), \\
\quad n_0(x) = \frac{ke^{-\alpha x}}{1+e^{-\alpha x}} \begin{cases} K & x \to -\infty \\ 0 & x \to +\infty \end{cases}
\end{cases}
$$

Case Study: Fisher's Equation

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```
> eq;
```

$$\frac{\partial}{\partial t} n(x, t) - d\left(\frac{\partial^2}{\partial x^2} n(x, t)\right) + \frac{r\, n(x, t)\, (-k + n(x, t))}{k}$$

Creating variables for the monomials of the input-output equation

```
> M1 := simplify(n(x, t)^2):
  M2 := simplify(diff(n(x, t), x, x)):
  M3 := simplify(n(x, t)):
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Creating the Wronskian of the monomials

```
> with(VectorCalculus):with(LinearAlgebra):
  Wr := simplify(Determinant(Wronskian([M1,M2,M3],x)));
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$$Wr := -\left(\frac{\partial^3}{\partial x^3} n(x, t)\right)\left(\frac{\partial^2}{\partial x^2} n(x, t)\right) n(x, t)^2 - 2\left(\frac{\partial^3}{\partial x^3} n(x, t)\right)\left(\frac{\partial}{\partial x} n(x, t)\right)^2 n(x, t) + 2\left(\frac{\partial^2}{\partial x^2} n(x, t)\right)\left(\frac{\partial}{\partial x} n(x, t)\right)^3 + \left(\frac{\partial}{\partial x} n(x, t)\right)\left(\frac{\partial^4}{\partial x^4} n(x, t)\right) n(x, t)^2$$

Case Study: Fisher's Equation

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Setting up differential algebra to study the Wronskian

```
> with(DifferentialAlgebra):
> R := DifferentialRing(blocks = [n], derivations = [x,t], arbitrary = [d,r,
  k]):
> RG := RosenfeldGroebner([eq], R); Equations(RG);
```

$$RG := [\mathit{regular\_differential\_chain}]$$

$$\left[\left[d\left(\frac{\partial^2}{\partial x^2} n(x,t)\right)k - \left(\frac{\partial}{\partial t} n(x,t)\right)k - r\, n(x,t)^2 + r\, n(x,t)\, k\right]\right] \quad ($$

Does the Wronskian vanish? Let us find out by computing the remainder modulo the IO-equation and listing the coefficients of the result as a polynomial in the parameters

```
> cf := coeffs(expand(numer(simplify(NormalForm(Wr, RG)))[1]),[k, r, d]);
```

$$cf := -2\left(\frac{\partial^2}{\partial t\partial x} n(x,t)\right)\left(\frac{\partial}{\partial x} n(x,t)\right)^2 n(x,t) + 2\left(\frac{\partial}{\partial x} n(x,t)\right)^3\left(\frac{\partial}{\partial t} n(x,t)\right), \left(\frac{\partial^2}{\partial t\partial x} n(x,t)\right) n(x, \quad (1$$

$$t)^3 - \left(\frac{\partial}{\partial x} n(x,t)\right)\left(\frac{\partial}{\partial t} n(x,t)\right) n(x,t)^2, -\left(\frac{\partial^2}{\partial t\partial x} n(x,t)\right) n(x,t)^4 + 2\left(\frac{\partial}{\partial x} n(x,t)\right)\left(\frac{\partial}{\partial t} n(x,$$

Case Study: Fisher's Equation


```
> Equations(RosenfeldGroebner([cf[-1],cf[1..4]],R));
```

$$\left[\left[\frac{\partial}{\partial x} n(x,t)\right], \left[\frac{\partial}{\partial t} n(x,t)\right]\right]$$

So if dn/dt <>0 and dn/dx<>0, then we have identifiability.

CASE 1. If dn/dx=0, then the PDE become the folling ODE:

```
> eqt := simplify(diff(n(t),t))- r*n(t) + (1/k)*(n(t))^2;
```

$$eqt := \frac{\mathrm{d}}{\mathrm{d}t} n(t) - r\, n(t) + \frac{n(t)^2}{k}$$

- This can be refuted using the fact that the initial condition does not depend on t.

Case Study: Fisher's Equation

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-------CASE 2. dn/dt=0:

```
> eqx := simplify(-d*diff(n(x),x$2) - r*n(x)+(1/k)*(n(x))^2);
```

$$eqx := -d\left(\frac{d^2}{dx^2}\,n(x)\right) - r\,n(x) + \frac{n(x)^2}{k} \quad (2$$

But at t=0, IC leads to describing n(x,t=0) in terms of exp:

```
> IC:=n(x)=simplify((k*exp(-a*x))/(1+exp(-a*x)));
```

$$IC := n(x) = \frac{k\,e^{-a x}}{1+e^{-a x}} \quad (2$$

```
> ICdiff:=simplify(diff(IC,x));
```

$$ICdiff := \frac{d}{dx}\,n(x) = -\frac{k\,a\,e^{-a x}}{\left(1+e^{-a x}\right)^2} \quad (2$$

Which can be plugged into (20), leading to:

```
> eqnx:=simplify(eval(eqx,IC));
```

$$eqnx := \frac{k\left(\left(d\,a^2 - 2\,r + 1\right)e^{-a x} + \left(-r+1\right)e^{-2 a x} - d\,a^2 - r\right)e^{-a x}}{\left(1+e^{-a x}\right)^3} \quad (2$$

This cannot happen because the latter expression must be zero according to the initial condition.

Case Study: Lotka Volterra Equation

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$$
\Sigma := \begin{cases}
\frac{\partial u(x,t)}{\partial t} - d_1 \frac{\partial u(x,t)}{\partial x^2} - u(x,t)(a_1 - b_1 u(x,t) - c_1 v(x,t)), \\
\frac{\partial v(x,t)}{\partial t} - d_2 \frac{\partial v(x,t)}{\partial x^2} - v(x,t)(a_2 - b_2 u(x,t) - c_2 v(x,t)) \\
-\infty < x < \infty, \quad 0 < t \\
\text{Boundary Cond.s:} \quad u(x,t) \to \begin{cases} \frac{a_1}{b_1} & x \to -\infty \\ 0 & x \to +\infty \end{cases} \\
\qquad\qquad\qquad\qquad v(x,t) \to \begin{cases} \frac{a_2}{c_2} & x \to -\infty \\ 0 & x \to +\infty \end{cases} \\
\text{Initial Cond.s:} \\
\quad u_0(x) = \frac{(a_1/b_1)e^{-\alpha_u x}}{1+e^{-\alpha_u x}} \begin{cases} a_1/a_2 & x \to -\infty \\ 0 & x \to +\infty \end{cases} \\
\quad v_0(x) = \frac{(a_1/b_1)e^{-\alpha_u x}}{1+e^{-\alpha_u x}} \begin{cases} a_1/a_2 & x \to -\infty \\ 0 & x \to +\infty \end{cases}
\end{cases}
$$

Case Study: Lotka Volterra Equation

```
> restart: with(DifferentialAlgebra): with(LinearAlgebra):
  sys := [
          diff(u(x, t), t) - d1 * diff(u(x, t), x$2) - u(x, t) * (a1 - b1 *
  u(x, t) - c1 * v(x, t)),
          diff(v(x, t), t) - d2 * diff(v(x, t), x$2) - v(x, t) * (a2 - b2 *
  u(x, t) - c2 * v(x, t)),
          y1(x, t) - u(x, t),
          y2(x, t) - v(x, t)
        ];
```

$$sys := \left[\frac{\partial}{\partial t} u(x,t) - d1 \left(\frac{\partial^2}{\partial x^2} u(x,t) \right) - u(x,t) \left(a1 - b1\, u(x,t) - c1\, v(x,t) \right), \frac{\partial}{\partial t} v(x,t) - d2 \left(\frac{\partial^2}{\partial x^2} v(x,t) \right) - v(x,t) \left(a2 - b2\, u(x,t) - c2\, v(x,t) \right), y1(x,t) - u(x,t), y2(x,t) - v(x,t) \right]$$

```
> R := DifferentialRing(blocks = [[u, v], [y1, y2]], derivations = [x, t],
  arbitrary = [a1, b1, c1, d1, a2, b2, c2, d2]):
> RG := RosenfeldGroebner(sys, R);
```

Case Study: Lotka Volterra Equation

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```
> IOeqs := Equations(RG[1])[-2..-1];
```

$$IOeqs := \left[\left(\frac{\partial^2}{\partial x^2} y1(x,t) \right) d1 - \frac{\partial}{\partial t} y1(x,t) - y1(x,t)^2 b1 - y1(x,t)\, y2(x,t)\, c1 + y1(x,t)\, a1, \left(\frac{\partial^2}{\partial x^2} y2(x,t) \right) d2 - \frac{\partial}{\partial t} y2(x,t) - y1(x,t)\, y2(x,t)\, b2 - y2(x,t)^2 c2 + y2(x,t)\, a2 \right]$$

```
> Ms1 := map2(coeff, IOeqs[1], [a1, b1, c1, d1], 1);
```

$$Ms1 := \left[y1(x,t), -y1(x,t)^2, -y1(x,t)\, y2(x,t), \frac{\partial^2}{\partial x^2} y1(x,t) \right]$$

```
> Ms2 := map2(coeff, IOeqs[2], [a2, b2, c2, d2], 1);
```

$$Ms2 := \left[y2(x,t), -y1(x,t)\, y2(x,t), -y2(x,t)^2, \frac{\partial^2}{\partial x^2} y2(x,t) \right]$$

```
> with(VectorCalculus):
> Wr1 := Wronskian(Ms1, x):
  Wr2 := Wronskian(Ms2, x):
```

Case Study: Lotka Volterra Equation


```
> R2 := DifferentialRing(blocks = [[y1, y2, u, v]], derivations = [x, t],
  arbitrary = [a1, b1, c1, d1, a2, b2, c2, d2]):
> RG2 := RosenfeldGroebner(sys, R2):
  Equations(RosenfeldGroebner(sys, R2));
```

$$\left[\left[d1\left(\frac{\partial^2}{\partial x^2}u(x,t)\right)-\frac{\partial}{\partial t}u(x,t)-u(x,t)^2\,b1-u(x,t)\,v(x,t)\,c1+u(x,t)\,a1,\ d2\left(\frac{\partial^2}{\partial x^2}v(x,t)\right)-\frac{\partial}{\partial t}\right.\right.$$

$$\left.\left. v(x,t)-u(x,t)\,v(x,t)\,b2-v(x,t)^2\,c2+v(x,t)\,a2,\ y1(x,t)-u(x,t),\ y2(x,t)-v(x,t)\right]\right]$$

```
> NF1 := NormalForm(simplify(Determinant(Wr1)), RG2):
> cfs := coeffs(expand(numer(NF1))[1], [a1, b1, c1, d1, a2, b2, c2, d2]):
> for cf in cfs do print(cf); print() od;
```

$$8\left(\frac{\partial}{\partial x}u(x,t)\right)^3\left(\frac{\partial}{\partial t}u(x,t)\right)\left(\frac{\partial}{\partial x}v(x,t)\right)u(x,t)\,v(x,t)-8\left(\frac{\partial^2}{\partial t\partial x}u(x,t)\right)\left(\frac{\partial}{\partial x}u(x,t)\right)^2\left(\frac{\partial}{\partial x}v(x,\right.$$

$$\left.t)\right)u(x,t)^2\,v(x,t)+2\left(\frac{\partial}{\partial x}u(x,t)\right)^2\left(\frac{\partial}{\partial t}u(x,t)\right)\left(\frac{\partial}{\partial x}v(x,t)\right)^2u(x,t)^2-2\left(\frac{\partial^2}{\partial t\partial x}u(x,t)\right)\left(\frac{\partial}{\partial x}\right.$$

Case Study: Lotka Volterra Equation

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```
> Equations(RosenfeldGroebner([cfs[-1],cfs[1..10]],R2));
```

$$\left[\left[\frac{\partial}{\partial t} u(x, t), \frac{\partial}{\partial t} v(x, t)\right], [v(x, t)], \left[\frac{\partial}{\partial x} u(x, t)\right]\right]$$

Case 2. $v(x, t) = 0$.

In contrast w the boundary condition $v \rightarrow \frac{a1}{b1}$ *when* $x \rightarrow$ infinity.

Case 3. $\frac{\partial}{\partial x} u(x, t)=0$

Contradicts because in this case u only depends on t, but the boundary conditions says u(x,0) varies (exponentially) with respect to alpha*x but we assume alpha non zero.

Case 1. $\frac{\partial}{\partial t} u(x, t) = 0$, $\frac{\partial}{\partial t} v(x, t) = 0$

Therefore $u = u(x)$ **and** $v = v(x)$ **and** *are given* **by** *the initial conditions* $u(x, 0)$ **and** $v(x, 0)$, *which are exponential functions. This means that We cannot say anything about identifiability.*