Structural and global identifiability for the classes of parametrized polynomial and parametrized rational systems

Jana Němcová and Jan H. van Schuppen

Centrum Wiskunde & Informatica, Amsterdam

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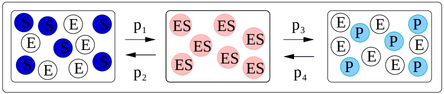
Rational systems and System identification

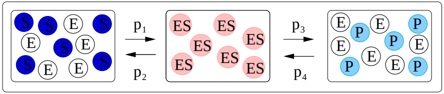


$$S + E \rightleftharpoons ES \rightleftharpoons P + E$$

$$\begin{aligned}
\dot{S} &= -p_1 S(E - ES) + p_2 ES \\
\dot{P} &= p_3 ES - p_4 ES(E - ES) \\
\dot{ES} &= p_1 S(E - ES) - (p_2 + p_3) ES + p_4 P(E - ES) \simeq 0
\end{aligned}$$

$$\begin{aligned}
\dot{S} &= \frac{-p_3 \frac{p_1}{p_2+p_3} E}{1 + \frac{p_1}{p_2+p_3} S + \frac{p_4}{p_2+p_3} P} S + \frac{p_2 \frac{p_4}{p_2+p_3} E}{1 + \frac{p_1}{p_2+p_3} S + \frac{p_4}{p_2+p_3} P} P \\
\dot{P} &= \frac{p_3 \frac{p_1}{p_2+p_3} E}{1 + \frac{p_1}{p_2+p_3} S + \frac{p_4}{p_2+p_3} P} S - \frac{p_2 \frac{p_4}{p_2+p_3} E}{1 + \frac{p_1}{p_2+p_3} S + \frac{p_4}{p_2+p_3} P} P
\end{aligned}$$

Rational systems and System identification



S + E ⇌ ES ⇌ P + E

$$
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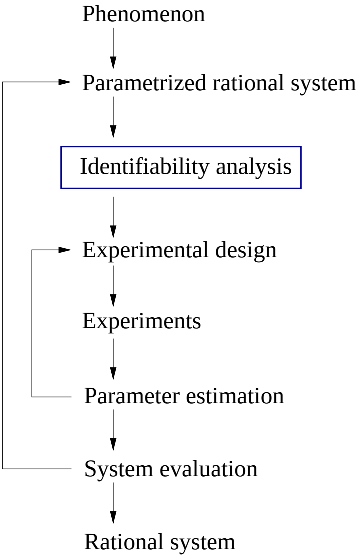
$$



Outline

Outline

Terminology

- **Irreducible real affine variety** X

  $X = \{(a_1,\ldots,a_n) \in \mathbb{R}^n | f_i(a_1,\ldots,a_n) = 0,\ f_i \in \mathbb{R}[X_1,\ldots,X_n], 1 \leq i \leq s\}$

- **Polynomial functions on** X

  $p : X \to \mathbb{R}$ is a polynomial on X if

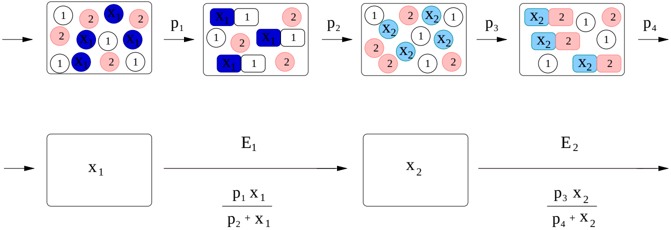
  $\exists\, f \in \mathbb{R}[X_1,\ldots,X_n]\, \forall\, (a_1,\ldots,a_n) \in X :\ p(a_1,\ldots,a_n) = f(a_1,\ldots,a_n)$

  $A = \{p \mid p - \text{polynomial on } X\}$ - finitely generated algebra

- **Rational functions on** X

  $Q = \{p/q \mid p, q \in A, q \neq 0\}$ - field of quotients of A

Example



$p_1, p_2, p_3, p_4 \in \mathbb{R}$ - fixed

$$
\left.\begin{aligned}
X &= \mathbb{R}^2 \\
\dot{x}_1 &= -\frac{p_1 x_1}{p_2 + x_1} + \alpha \\
\dot{x}_2 &= \frac{p_1 x_1}{p_2 + x_1} - \frac{p_3 x_2}{p_4 + x_2}
\end{aligned}\right\} \quad f_\alpha = \left(-\frac{p_1 x_1}{p_2 + x_1} + \alpha\right)\frac{\partial}{\partial x_1} + \left(\frac{p_1 x_1}{p_2 + x_1} - \frac{p_3 x_2}{p_4 + x_2}\right)\frac{\partial}{\partial x_2}
$$

$$
y = h(x_1, x_2) = \left(\frac{p_1 x_1}{p_2 + x_1}, \frac{p_3 x_2}{p_4 + x_2}\right)^T
$$

$$
x_1(0) = x_2(0) = 1
$$

Rational systems

- the input space $U \subseteq \mathbb{R}^m$
- the space of input functions

$$\mathcal{U}_{pc} = \{u : [0,\infty) \to U \mid u \text{ piecewise constant}\}$$

$$u = (\alpha_1, t_1) \dots (\alpha_k, t_k) \in \mathcal{U}_{pc},\ \alpha_i \in U$$

- the output space $\mathbb{R}^r$

A rational system Σ is a quadruple (X, f, h, x_0) where

- X is an irreducible real affine variety,
- $f = \{f_\alpha | \alpha \in U\}$ is a family of rational vector fields on X,
- $h : X \to \mathbb{R}^r$ is an output map with rational components,
- $x_0 \in X$ is an initial state.

Reachability and observability

Definition

A rational system $\Sigma = (X, f = \{f_\alpha | \alpha \in U\}, h)$ is

- algebraically reachable from $x_0 \in X$ if

$$\mathcal{R}(x_0) = \{x_\Sigma(T_u; x_0, u) \in X | u \in \mathcal{U}_{pc}(\Sigma)\} \text{ is Z-dense in } X,$$

- rationally observable if $Q_{obs}(\Sigma) = Q$.

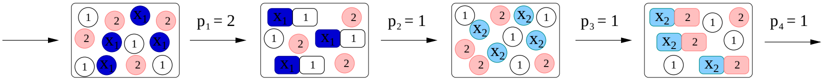
observation algebra

$$A_{obs}(\Sigma) = \mathbb{R}[\{h, f_{\alpha_1,\ldots,\alpha_i} h \mid i \in \mathbb{N}, \alpha_j \in U, j = 1,\ldots,i\}]$$

observation field

$$Q_{obs}(\Sigma) = Q_{obs}(\Sigma) = \{p/q \mid p,q \in A_{obs}(\Sigma), q \neq 0\}$$

Example



$$X = \mathbb{R}^2 \qquad f_\alpha = \left(\frac{-2x_1}{1+x_1} + \alpha\right)\frac{\partial}{\partial x_1} + \left(\frac{2x_1}{1+x_1} - \frac{x_2}{1+x_2}\right)\frac{\partial}{\partial x_2}$$

$$x_1(0) = x_2(0) = 1 \qquad h(x_1, x_2) = \left(\frac{2x_1}{1+x_1}, \frac{x_2}{1+x_2}\right)^T$$

Algebraic reachability

$$C = \mathrm{span}\{[X_k, [\ldots, [X_2, X_1]\ldots]]\},\ X_1 = \begin{pmatrix}1\\0\end{pmatrix},\ X_{\geq 2} \in \left\{\begin{pmatrix}\frac{-2x_1}{1+x_1}\\ \frac{2x_1}{1+x_1} - \frac{x_2}{1+x_2}\end{pmatrix}, \begin{pmatrix}1\\0\end{pmatrix}\right\}$$

$$\dim C((x_1(0), x_2(0))) = \dim\begin{pmatrix}-1 & 1\\ 1 & 0\end{pmatrix} = 2$$

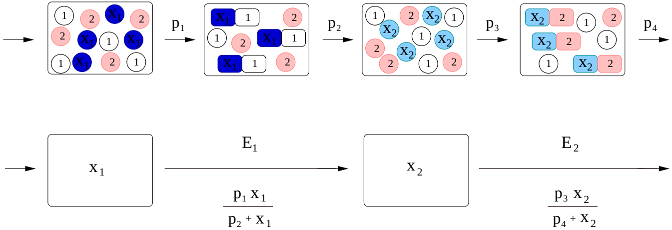
Rational observability

$$Q_{obs}(\Sigma) = \mathbb{R}(h_1, h_2, f_\alpha h_1, f_\alpha h_2, \ldots)$$

$$h_1 = \frac{2x_1}{1+x_1},\ f_\alpha h_1 = (-h_1 + \alpha)\frac{2}{(1+x_1)^2} \Rightarrow (1+x_1)^2,\ x_1^2 \in Q_{obs}(\Sigma) \Rightarrow x_i \in Q_{obs}(\Sigma)$$

Outline

Example



$p_1, p_2, p_3, p_4 \in \mathbb{R}$ - variables

$$\left.\begin{array}{l} X^p = \mathbb{R}^2 \\ f_\alpha^p = \left(-\frac{p_1 x_1}{p_2 + x_1} + \alpha\right)\frac{\partial}{\partial x_1} + \left(\frac{p_1 x_1}{p_2 + x_1} - \frac{p_3 x_2}{p_4 + x_2}\right)\frac{\partial}{\partial x_2} \\ h^p(x_1, x_2) = \left(\frac{p_1 x_1}{p_2 + x_1}, \frac{p_3 x_2}{p_4 + x_2}\right)^T \\ x_1^p(0) = x_2^p(0) = 1 \end{array}\right\} \quad \Sigma(p),\ p \in \mathbb{R}^4$$

Parametrized systems

Parametrized rational system $\Sigma(P)=\{\Sigma(p)=(X^p,f^p,h^p,x_0^p)|p\in P\}$:

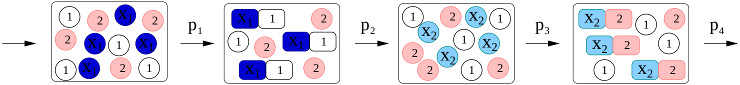
- $P\subseteq\mathbb{R}^s$ an irreducible variety - parameter set
- the same input spaces $U\subseteq\mathbb{R}^m$ and output spaces $\mathbb{R}^r$
- $X^p\neq X^{p'}$

Properties:

- structural reachability: $Z\text{-}cl(\mathcal{R}(x_0^p))=X^p$ for all $p\in P\setminus C$
- structural observability: $Q_{obs}(\Sigma(p))=Q^p$ for all $p\in P\setminus O$
- structural canonicity: $\Sigma(p)$ is algebraically reachable and rationally observable for all $p\in P\setminus CO$
- structurally distinguishes parameters: $\mathbb{R}(\{q^{f_\alpha}_{k,i;a^k_1,\dots,a^k_{n_p}},q^{h}_{k,j;b^k_1,\dots,b^k_{n_p}},q_i^{x_0}\})\cong Q^P$ for all $p\in P\setminus D$

$$\left.\begin{array}{l}\dot{x}=p^2x\\ x(0)=1\end{array}\right\}\quad\Rightarrow\quad\text{the same solution for } p,-p$$

Example



$$\Sigma(p),\ p \in P = \mathbb{R}^4 : \quad \begin{cases} X^p = \mathbb{R}^2 \\ f^p_\alpha = \frac{p_2\alpha+(\alpha-p_1)x_1}{p_2+x_1}\frac{\partial}{\partial x_1} + \frac{p_1p_4x_1-p_2p_3x_2+(p_1-p_3)x_1x_2}{p_2p_4+p_4x_1+p_2x_2+x_1x_2}\frac{\partial}{\partial x_2} \\ h^p(x_1,x_2) = \left(\frac{p_1x_1}{p_2+x_1}, \frac{p_3x_2}{p_4+x_2}\right)^T \\ x_1^p(0) = x_2^p(0) = 1 \end{cases}$$

$\Sigma(P)$ is structurally canonical :

$$CO = \{p \in \mathbb{R}^4 | (p_1p_2p_3p_4)(p_2+1)(p_4+1)(p_1(p_4+1)-p_3(p_2+1)) = 0\}$$

$\Sigma(P)$ structurally distinguishes parameters : $D = \{p \in \mathbb{R}^4 | p_1p_2p_3p_4 = 0\}$

$$\mathbb{R}[\ \overbrace{p_2\alpha, \alpha-p_1, p_2, 1}^{f^p_{\alpha,1}:\ q^{f\alpha}_{1;0,0}, q^{f\alpha}_{1;1,0}, q^{f\alpha}_{2;0,0}, q^{f\alpha}_{2;0,1}}\ , \overbrace{p_1p_4, \ldots, 1}^{f^p_{\alpha,2}}, \overbrace{p_3, p_4, 1}^{h^p}, \overbrace{1}^{x_0^p}\ ] = \mathbb{R}[p_1,p_2,p_3,p_4] = A^P$$

Structured systems

$\Sigma(p), \Sigma(\overline{p}) \in \Sigma(P)$ are birationally equivalent if

- $X^p, X^{\overline{p}}$ birationally equivalent
  $\exists \phi : X^p \to X^{\overline{p}}$, $\psi : X^{\overline{p}} \to X^p$ rational s.t. $\phi \circ \psi = 1_{X^{\overline{p}}}, \psi \circ \phi = 1_{X^p}$
- $\forall \varphi \in Q^{\overline{p}}, \forall \alpha \in U : f^p_\alpha(\varphi \circ \phi) = (f^{\overline{p}}_\alpha \varphi) \circ \phi$
- $h^{\overline{p}} \circ \phi = h^p$
- ϕ defined at x^p_0, and $\phi(x^p_0) = x^{\overline{p}}_0$

$\Sigma(P)$ is a structured system if for every $p, \overline{p} \in P$:

- $X^p, X^{\overline{p}}$ birationally equivalent
- "$p = \overline{p}$" $\Rightarrow \Sigma(p), \Sigma(\overline{p})$ birationally equivalent

Structured systems - example

$$\Sigma(P) = \{\Sigma(p) | p = (p_1, p_2, p_3, p_4) \in P = \mathbb{R}^4\}$$

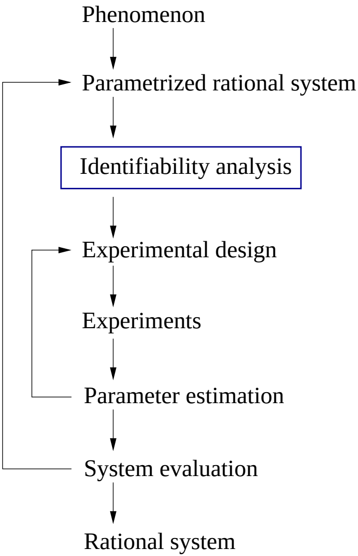
$$\left.\begin{array}{l} X^p = \mathbb{R}^2 \\ f^p_\alpha = \left(\frac{-p_1 x_1}{p_2 + x_1} + \alpha\right)\frac{\partial}{\partial x_1} + \left(\frac{p_1 x_1}{p_2 + x_1} - \frac{p_3 x_2}{p_4 + x_2}\right)\frac{\partial}{\partial x_2} \\ h^p(x_1, x_2) = \left(\frac{p_1 x_1}{p_2 + x_1}, \frac{p_3 x_2}{p_4 + x_2}\right)^T \\ x^p_1(0) = x^p_2(0) = 1 \end{array}\right\} \Rightarrow \quad \begin{array}{l} \Sigma(P) \text{ structured} \\ \phi = id \end{array}$$

$\overline{p} \in P$

$$\left.\begin{array}{l} X^{\overline{p}} = \{(x_1, x_2, x_3) \in \mathbb{R}^3 | x_1^2 + x_2^2 + x_3^2 - 1 = 0\} \\ f^{\overline{p}}_\alpha = f^{\overline{p}}_{\alpha,1}\frac{\partial}{\partial x_1} + f^{\overline{p}}_{\alpha,2}\frac{\partial}{\partial x_2} + f^{\overline{p}}_{\alpha,3}\frac{\partial}{\partial x_3} \\ h^{\overline{p}}(x_1, x_2, x_3) = \left(\frac{\overline{p_1} x_1}{\overline{p_2} + x_1 - \overline{p_2} x_3}, \frac{\overline{p_3} x_2}{\overline{p_4} + x_2 - \overline{p_3} x_3}\right)^T \\ x^{\overline{p}}_1(0) = x^{\overline{p}}_2(0) = \frac{2}{3}, x^{\overline{p}}_3(0) = \frac{1}{3} \end{array}\right\} \Rightarrow \quad \begin{array}{l} \Sigma(\overline{p}) \overset{\phi}{\longleftrightarrow} \Sigma(p) \\ \phi : X^{\overline{p}} \to X^p \\ \phi(x_1, x_2, x_3) = \\ \qquad \left(\frac{x_1}{1 - x_3}, \frac{x_2}{1 - x_3}\right) \end{array}$$

Outline

Can the parameters be determined uniquely?



Assumption: $\forall p \in P : \widetilde{\mathcal{U}_{pc}} \subseteq \mathcal{U}_{pc}(\Sigma(p))$

A parametrization $\mathcal{P} : P \to \Sigma(P)$ is

- globally identifiable if

  $$p \mapsto \{(u, h^p(x^p(T_u; x_0^p, u))) | u \in \widetilde{\mathcal{U}_{pc}}\}$$

  is injective on P
- structurally identifiable if

  $$p \mapsto \{(u, h^p(x^p(T_u; x_0^p, u))) | u \in \widetilde{\mathcal{U}_{pc}}\}$$

  is injective on $P \setminus S \neq \emptyset$

Structural and global identifiability

Theorem

Let $\Sigma(P)$ be a structured rational system which

- *is structurally canonical ($CO \subsetneq P$ the smallest variety s.t. $\Sigma(p)$ is canonical for all $p \in P \setminus CO$), and*
- *structurally distinguishes parameters (with $D \subsetneq P$ the smallest).*

Then the following are equivalent:

- $\mathcal{P} : P \to \Sigma(P)$ *is structurally identifiable (with S)*
- $\exists G : CO \cup D \subseteq G \subsetneq P \; \forall p, \overline{p} \in P \setminus G : \quad \Sigma(p) \xleftrightarrow{id} \Sigma(\overline{p})$

global identifiability:

- polynomial systems $CO, D, S, G = \emptyset$
- rational systems $CO, D, S, G = W$

Proof

$\mathcal{P}$ structurally identifiable (with S) $\Rightarrow \exists G\ \forall p,\overline{p} \in P \setminus G : \Sigma(p) \overset{id}{\longleftrightarrow} \Sigma(\overline{p})$

$S \subsetneq P : p \mapsto \{(u, h^p(x^p(T_u; x_0^p, u))) | u \in \widetilde{\mathcal{U}_{pc}}\}$ injective on $P \setminus S$
$G = CO \cup D \cup S \rightsquigarrow G \subsetneq P$

$p,\overline{p} \in P \setminus G \Rightarrow \Sigma(p), \Sigma(\overline{p})$ canonical + realizing the same data
(realization theory) $\Rightarrow$ birationally equivalent *(observability)* $\Rightarrow \phi$ identity

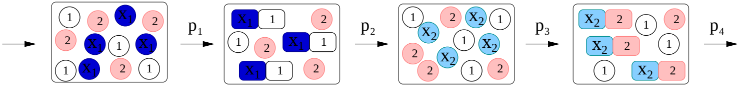
$\exists G\ \forall p,\overline{p} \in P \setminus G : \Sigma(p) \overset{id}{\longleftrightarrow} \Sigma(\overline{p}) \Rightarrow \mathcal{P}$ structurally identifiable (with S)

$S = G,\ p,\overline{p} \in P \setminus S$ *(realization theory + reachability)* $\Rightarrow$

$$X^p = X^{\overline{p}} \rightsquigarrow Q^p = Q^{\overline{p}}$$
$$\forall \varphi \in Q^{\overline{p}},\ \forall \alpha \in U : f_\alpha^p \varphi = f_\alpha^{\overline{p}} \varphi$$
$$h^p = h^{\overline{p}}$$
$$x_0^p = x_0^{\overline{p}}$$

(distinguishing parameters) $\Rightarrow p = \overline{p}$

Example (1)



$$\Sigma(P) = \{\Sigma(p) = (X^p, f^p, h^p, x_0^p) | p = (p_1, p_2, p_3, p_4) \in P = \mathbb{R}^4\}$$

- structured rational system
- structurally canonical
- structurally distinguishes parameters

Theorem:

$\mathcal{P} : P \to \Sigma(P)$ is structurally identifiable $\Leftrightarrow$ $\forall p, \overline{p} \in P \setminus (CO \cup D)$: $\left(\Sigma(p) \overset{\phi}{\longleftrightarrow} \Sigma(\overline{p}) \Rightarrow \phi \text{ identity}\right)$

Example (2)

$$\left.\begin{array}{l} p,\overline{p} \in \underbrace{P \setminus (CO \cup D)} \Rightarrow \Sigma(p), \Sigma(\overline{p}) \text{ canonical} \\ \forall u \in \widetilde{\mathcal{U}}_{pc} :\ h^p(x^p(T_u; x_0, u)) = h^{\overline{p}}(x^{\overline{p}}(T_u; x_0, u)) \end{array}\right. \Rightarrow \begin{array}{l}\Sigma(p), \Sigma(\overline{p}) \\ \text{birationally} \\ \text{equivalent}\end{array}$$

$$\Sigma(p) \overset{\phi}{\longleftrightarrow} \Sigma(\overline{p}) \rightsquigarrow \phi = (\phi_1, \phi_2) : \mathbb{R}^2 \to \mathbb{R}^2$$

(i) $\forall \varphi \in \mathbb{R}(X_1, X_2), \forall \alpha \in \mathbb{R} : f^p_\alpha(\varphi \circ \phi) = (f^{\overline{p}}_\alpha \varphi) \circ \phi$

(ii) $h^{\overline{p}} \phi = h^p$

(iii) $\phi(x^p_0) = x^{\overline{p}}_0$

- (ii) $\Rightarrow \frac{\overline{p_1}\phi_1(x_1,x_2)}{\overline{p_2}+\phi_1(x_1,x_2)} = \frac{p_1 x_1}{p_2 + x_1}, \ \frac{\overline{p_3}\phi_2(x_1,x_2)}{\overline{p_4}+\phi_2(x_1,x_2)} = \frac{p_3 x_2}{p_4 + x_2}$
- (i) + ($\varphi(x_1, x_2) = x_1$) + (ii) + (iii) $\Rightarrow \phi_1(x_1, x_2) = x_1$
- (i) + ($\varphi(x_1, x_2) = x_2$) + (ii) + (iii) $\Rightarrow \phi_2(x_1, x_2) = x_2$

$\Rightarrow \phi(x_1, x_2) = (x_1, x_2) \Rightarrow \mathcal{P} : P \to \Sigma(P)$ structurally identifiable

Concluding remarks

Results

- Structural and global identifiability
- Application to biology

Further research

- Structural distinguishability
- Determining numerical values of parameters
- Excitation of inputs
- Computational methods

Acknowledgements

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