# Applications of computer algebra in the identifiability and diagnosability studies

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# Outline

The relative identifiability

- State of the problem
- A short quiz
- A first neuron model
- Formalization of the identifiability definition
- Towards the relative identifiability with a (little) more complex example

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- Conclusion
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- Fault diagnosability
- State of the problem
- Algebraic signature
- Characterization of a single fault/Expected values of ASig
- Conclusion

#### Tutorial

- Relative identifiability
- Diagnosability



# Considered model

Given a system or a process, some quantities interact:





# Neuron responding to a electrical signal

- Electrical signal (*I*)
- Membrane potential (V)
- Perturbations
- Non measurable varying quantities
- Unknown constant values

# Schematic representation of the functioning of the neuron

$$u = l = input$$

$$y = V = output$$

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xp = vector of unknown parameters.

# Considered model

Given a system or a process, some quantities interact:





# Neuron responding to a electrical signal

Schematic representation of the functioning of the neuron

$$\begin{cases} \dot{x}(t,p) = f(x(t,p), u(t), p), \\ y(t,p) = h(x(t,p), p). \end{cases}$$
(1)

- $\checkmark$  f, h: real functions, analytic on M (an open set of  $\mathbb{R}^n$ ),
- $\begin{array}{l} \checkmark \quad p \in \mathcal{U}_{\mathcal{P}} \colon \text{vector of parameters,} \\ \mathcal{U}_{\mathcal{P}} \subset \mathbb{R}^{r} : \text{ an a priori known set of admissible parameters.} \end{array}$

Assume that the process can be modeled by

 $\begin{cases} \dot{x}(t,p) = f(x(t,p), u(t), p), \\ y(t,p) = h(x(t,p), p). \end{cases}$ 

Two problems can be considered:

- $\checkmark$  The forward problem: given p, u, find x and y.
- ✓ The inverse problem: given y and u, estimate p.



Identifiability problem

#### Question

From the output(s) of the system, is it possible to estimate uniquely the parameter vector p?

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If the answer is YES, then the model is said identifiable.



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Two problems can be considered:

- $\checkmark$  The forward problem: given p, u, find x and y.
- $\checkmark$  The *inverse problem*: given y and u, estimate p.

A property of lots of inverse problems: *ill-posedness*.

#### Well-posedness is the sense of Hadamard

A problem is said well-posed in the sense of Hadamard if it satisfies the following properties:

- Existence: For all (suitable) data, there exists a solution of the problem (in an appropriate sense)
- 2 Unicity : for all available data, the solution is unique
  - Stability : the solution depends continuously of the data.

Example: The differentiation and integration are two inverse problems of each other.

- $\checkmark$  Microscopic worm Caenorhabditis elegans ( $\approx 1 mm$  de long) has .... neurons
- ✓ The insects have approximatively ..... of neurons
- ✓ Modern man has ...... of neurons in its best form
- ✓ Every day we loose approximatively ..... neurons, which is the equivalent of .....

- $\checkmark$  At 80 years old, the brain is only ..... percent of what it was around 20 years
- ✓ Nerve information passes from neurons to neurons, up to .....

- $\checkmark$  Microscopic worm Caenorhabditis elegans ( $\approx 1 mm$  de long) has 302 neurons
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- ✓ At 80 years old, the brain is only 70 percent of what it was around 20 years
- ✓ Nerve information passes from neurons to neurons, up to 120 m / s, ie 430 km / h.

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#### Neuron

A neuron is a nerve cell, that is an electrically excitable cell that receives, processes, and transmits information through electrical and chemical signals.



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### Membrane

#### A lipid membrane

A membrane is composed of a lipid bilayer which separates the intracellular milieu and the extracellular milieu.



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The main ions in a neuron are:

- Sodium (*Na*<sup>+</sup>)
- Potassium ( $K^+$ )
- Calcium ( $Ca^{2+}$ )
- Chlorure (Cl<sup>-</sup>)



Unequally distribution of ions

on both sides of the membrane

- Specific channels for each ion
- Channels can be:
  - ✓ open or close
  - ✓ active or inactive.

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However there is electroneutrality!



Some mechanisms permit to regulate ionic concentrations and to maintain them constant. Two types of transport:

- ✓ passive transport:
  - the concentration gradient: ions go from the most concentrated milieu to the least concentrated milieu extracellular → intracellular: Cl<sup>-</sup>, Na<sup>+</sup>, Ca<sup>2+</sup> intracellular → extracellular: K<sup>+</sup>
  - electrical gradient: the membrane is electrically charged: negatively inside, positively outside extracellular  $\rightarrow$  intracellular:  $K^+$ ,  $Na^+$  et  $Ca^{2+}$  are attracted inside the neuron intracellular  $\rightarrow$  extracellular:  $Cl^-$

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active transport (NA/K pump) requiring energy.



Potential differences:



Modeling of a simple ion channel with one activation (m):

I = G(V - E) where G = gm

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where

- V (mV): voltage
- g(nS): maximal conductance
- E(mV): equilibrium potential
- *m* is the probability of a canal to be open

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- E(mV): equilibrium potential
- *m* is the probability of a canal to be open

The equation describing the activation of the gates to the answer of the potential of membrane is

$$\frac{dm}{dt} = \frac{m_{\infty}(V) - m}{\tau(V)}$$

where

- $m_{\infty}(V)$ : the equilibrium value of m,
- $\tau(V)$ : times at which the equilibrium is attained.

#### Question

Is it possible to determine in a unique way  $m_{\infty}$  , au , g from the measurement of the current?

## What can we measure?

The voltage-clamp protocol

- Characterizes the activation or inactivation properties of the ionic canal
- necessitates to treat the membrane of the neuron (tetrodoxine)
- consists in holding the voltage (= V) piecewise constant  $\hookrightarrow$  after a while,  $m_{\infty}$ ,  $\tau$  can be considered as constant and we have

$$\frac{dm}{dt} = \frac{m_{\infty} - m}{\tau}$$

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Assumptions

 $\checkmark$  V = constant input

$$\checkmark$$
 *I* = output (= *y*)

 $\checkmark$  m = state variable (= x)

A first example: The equation of one ion channel with one activation variable:

$$\begin{cases} I = g m (V - E) \\ \frac{dm}{dt} = \frac{m_{\infty} - m}{\tau} & \underset{y:=l}{\longleftrightarrow V-E=cst}, \end{cases} \begin{cases} y = g m u \\ \frac{dm}{dt} = \frac{m_{\infty} - m}{\tau} \end{cases}$$

Controlled models ( $u \neq 0$ ) WITHOUT initial condition; ( $\bar{x}, \bar{y}$ ) = unique set of solutions

• The model is **globally identifiable** if there exists an input *u* such that, for all  $p \in U_p$ , one gets

$$\left. \begin{array}{c} \bar{y}(t,\rho) \neq \emptyset, \\ \bar{y}(t,\rho) \cap \bar{y}(t,\bar{\rho}) \neq \emptyset, \ \forall \ t \ge 0, \ \bar{\rho} \in \mathcal{U}_{\rho} \end{array} \right\} \quad \Rightarrow \quad \rho = \bar{\rho}. \tag{2}$$

• The model is **locally identifiable** if it is globally identifiable in an open neighborhood  $v(p) \subset U_p$  of p.

#### Proposition

If V is a constant input and I is an output of the model then the model is not identifiable, in particular with respect to  $\tau$  and  $m_{\infty}$ .

#### Proof.

A first example: The equation of one ion channel with one activation variable:

$$\begin{cases} I = gm(V-E) \\ \frac{dm}{dt} = \frac{m_{\infty} - m}{\tau} & \underset{y:=l}{\longleftrightarrow V \in E=cst}, \end{cases} \begin{cases} y = gmu \\ \frac{dm}{dt} = \frac{m_{\infty} - m}{\tau} \end{cases}$$

Concretely



The model can produce exactly the same output for different parameter/initial condition values!

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A first example: The equation of one ion channel with one activation variable:

$$\begin{cases} l = gm(V-E) \\ \frac{dm}{dt} = \frac{m_{\infty} - m}{\tau} & \stackrel{\longleftrightarrow}{\underset{u:=V \in E = cst,}{\longleftrightarrow}} \\ m(0) = m_0 & y:=l \end{cases} \begin{cases} y = gmu \\ m = m_{\infty} + (m_0 - m_{\infty})e^{-\frac{t}{\tau}} \end{cases}$$

#### Controlled model ( $u \neq 0$ ) WITH initial conditions; (x, y) unique solution

- The model is **globally identifiable** if there exists an input *u* such that, for all  $p, \bar{p} \in U_p$ , there exists  $t_1 > 0$  such that if for all  $t \in [0, t_1]$ , the equalities  $y(t, p) = y(t, \bar{p})$  implies that  $p = \bar{p}$ .
- The model is **locally identifiable** if it is globally in an open neighborhood  $v(p) \subset U_p$  of p.

#### Proposition

If V is a constant input and I is an output of the model then the model is identifiable, in particular au and  $m_{\infty}$ .

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#### Proof.

#### Summary

- ✓ Identifiability: based on specific relations called Input-Output (IO) polynomials.
- $\checkmark$  The Rosenfeld-Groebner algorithm permits to obtain them. They take the form

$$P(y, u, p) = m_0(y, u) + \sum_{k=1}^{r} \gamma_k(p) m_k(y, u) = 0.$$

✓ If  $(m_k(y, u))_{k=1,...,q}$  are linearly independent, the model is globally identifiable at p if for all  $\bar{p} \in U_p$ 

$$\forall k = 1, \dots, q, \ \gamma_k(\bar{p}) = \gamma_k(p) \Rightarrow p = \bar{p}.$$
(3)

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- ✓ If  $\phi(p) = (\gamma_k(p))_{k=1,...,q}$ , (3) consists in verifying that  $\phi$  is injective.
- Initial conditions can be introduced with algebraic relations.

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A (little) more complex example....

$$\begin{cases} I = gmh(V - E), \\ \frac{dm}{dt} = \frac{m_{\infty} - m}{\tau_m}, \\ \frac{dh}{dt} = \frac{h_{\infty} - h}{\tau_h}, \\ p_1 = \frac{1}{\tau_m}, p_2 = m_{\infty}, \\ p_3 = \frac{1}{\tau_h}, p_4 = h_{\infty}, p_5 = g, \end{cases} \begin{cases} y = up_5 x_1 x_2, \\ \dot{x}_1 = p_1 (p_2 - x_1), \\ \dot{x}_2 = p_3 (p_4 - x_2). \end{cases}$$

Non identifiable model!

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Questions :

- X Key parameters permitting to obtain the identifiability of one or some non measurable parameters and eventually the identifiability of the model?
- X Roles of the constraints?
- X Natural integration of the constraints or the initial conditions in the identifiability study?

The relative identifiability complex example

$$\begin{array}{l} I = gmh(V - E), \\ \frac{dm}{dt} = \frac{m_{\infty} - m}{\tau_m}, \\ \frac{dh}{dt} = \frac{h_{\infty} - h}{\tau_h}, \end{array} \iff \begin{cases} y = u p_5 x_1 x_2, \\ \dot{x}_1 = p_1 (p_2 - x_1), \\ \dot{x}_2 = p_3 (p_4 - x_2). \end{cases}$$



Obtain from  $\phi$  and a set of algebraic constraints a **decision tree**!

The relative identifiability complex example

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First step: Redefine the identifiability: Relative identifiability For example:



- $p_1$  is not identifiable;
- *p*<sub>3</sub> is relatively identifiable with respect to the set {*p*<sub>1</sub>};
- *p*<sub>5</sub> relatively identifiable with respect to the set {*p*<sub>1</sub>, *p*<sub>3</sub>};
- p<sub>2</sub> and p<sub>4</sub> are not relatively identifiable with respect to the set {p<sub>1</sub>, p<sub>3</sub>}.

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$$\begin{array}{l} I = gmh(V - E), \\ \frac{dm}{dt} = \frac{m_{\infty} - m}{\tau_m}, \\ \frac{dh}{dt} = \frac{h_{\infty} - h}{\tau_h}, \end{array} \iff \begin{cases} y = u p_5 x_1 x_2, \\ \dot{x}_1 = p_1 (p_2 - x_1), \\ \dot{x}_2 = p_3 (p_4 - x_2). \end{cases}$$

Second step: definition of a semi-algebraic set from

•  $\phi(p) = (\gamma_k(p))_{k=1,...,9}$  the coefficient vector of the IO polynomial:

$$\ddot{y}^{2} + \gamma_{1}y^{2} + \gamma_{2}y\dot{y} + \gamma_{3}y\ddot{y} + \gamma_{4}y + \gamma_{5}\dot{y}^{2} + \gamma_{6}\dot{y}\ddot{y} + \gamma_{7}\dot{y} - \gamma_{8}\ddot{y} + \gamma_{9} = 0$$
(4)

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 C the semi-algebraic set defined by C(p) composed of all algebraic equations and inequalities verified by the components of the parameter vector p = (p<sub>1</sub>,..., p<sub>5</sub>)

to test

$$\begin{cases} \begin{array}{ll} p \in \mathcal{C} \\ \bar{p} \in \mathcal{C} \\ p_1 & = \bar{p}_1, \\ p_3 & = \bar{p}_3, \\ \phi(p) & = \phi(\bar{p}) \end{array} \Rightarrow p_5 = \bar{p}_5. \end{cases}$$

$$\begin{array}{l} I = gmh(V - E), \\ \frac{dm}{dt} = \frac{m_{\infty} - m}{\tau_m}, \\ \frac{dh}{dt} = \frac{h_{\infty} - h}{\tau_h}, \end{array} \iff \begin{cases} y = u p_5 x_1 x_2, \\ \dot{x}_1 = p_1 (p_2 - x_1), \\ \dot{x}_2 = p_3 (p_4 - x_2). \end{cases}$$

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to test

 $S_{p_1,p_3} \cup \{p_5 \neq \overline{p}_5\}$  has no real solution.

where

 $S_{p_1,p_3} = C(p) \cup C(\bar{p}) \cup \{p_1 = \bar{p}_1, p_3 = \bar{p}_3\} \cup \{\gamma_k(p) = \gamma_k(\bar{p}) \mid k = 1, \dots, 9\}.$ 

 $\implies$  development of a method and the algorithm *IdentifiabilityTree*.

$$\begin{cases}
I = gmh(V - E), \\
\frac{dm}{dt} = \frac{m_{\infty} - m}{\tau_m}, \\
\frac{dh}{dt} = \frac{h_{\infty} - h}{\tau_h}, \\
p_1 = \frac{1}{\tau_m}, p_2 = m_{\infty}, \\
p_3 = \frac{1}{\tau_h}, p_4 = h_{\infty}, p_5 = g,
\end{cases}
\begin{cases}
y = u p_5 x_1 x_2, \\
\dot{x}_1 = p_1 (p_2 - x_1), \\
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\end{cases}$$

#### Results of the IdentifiabilityTree algorithm:

- One of the branch:  $[p_2, p_4, p_5, p_3, p_1]$
- Two groups of parameters  $\{p_2, p_4, p_5\}$  and  $\{p_1, p_3\}$ .
- Determination of the two parameters p<sub>2</sub>, p<sub>4</sub> and the parameter p<sub>3</sub> ensures the identifiability of all the parameters.

#### The voltage clamp experiment:

- Estimate the triplet  $\{p_2, p_4, p_5\}$  from  $y = up_5 x_1 x_2$  in fixing the voltage at different values and measuring the transmembrane current trace (*V* constant:  $I = (V E)p_5 p_2 p_4$ );
  - Estimate  $p_1$  and  $p_3$  at a particular voltage value dependence.

#### Conclusion

Identifiability study:

- ✓ Ensures good properties to the mathematical model;
- ✓ Extension of this definition;
- ✓ Other examples: strategy to reparametrize unidentifiable ODE models into identifiable ones (Evans 2000, Meshkat 2011)....

The models

$$\begin{cases} \dot{x}(t, p, f) = g(x(t, p), u(t), f, p), \\ y(t, p, f) = h(x(t, p), u(t), f, p), \\ x(t_0, p, f) = x_0, \\ t_0 \le t \le T. \end{cases}$$
(6)

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#### Definitions

- ✓ A fault is an unpermitted deviation of at least one parameter of the system from the acceptable standard condition.
- ✓ Fault diagnosability establishes which faults can be discriminated using the available sensors in a system.
- ✓ Fault diagnosis consists in fault detection of the malfunction of a system and the fault isolation of the faulty component.

f = 0 means no fault. In the case of uncontrolled models u = 0.

Example: Mass (m = 1) attached to an elastic spring (force k) u external force ( $\neq 0$ ),  $d \ge 1$ 

$$\ddot{y} + k(f_1 - 1)^2 y - (d + f_2)u = 0$$
  $\phi(f) = \left(k(f_1 - 1)^2, -d - f_2\right)$ 

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Algebraic signature

$$\begin{split} &ASig(f) = \left(k(f_1 - 1)^2, -d - f_2\right), \text{ in particular:} \\ &\textbf{\textit{X}} \ ASig(f_{\{1\}}) = \left(k(f_1 - 1)^2, -d\right) \text{ et } ASig(f_{\{1,2\}}) = \left(k(f_1 - 1)^2, -d - f_2\right), \\ &\textbf{\textit{X}} \ ASig(f_{\{1\}}) \cap ASig(f_{\{1,2\}}) = \emptyset \text{ for all } f_2 \in (0,2), -d \neq -d - f_2. \end{split}$$

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#### Definitions

X Two sets of faults are said algebraic discriminable if there exists an algebraic signature, such that, for all input u, the two signatures have an empty intersection.

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X If all the distinct sets of faults are algebraic discriminable, the model is said algebraically diagnosable.

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#### Definitions

- X Two sets of faults are said **algebraic discriminable** if there exists an algebraic signature, such that, for all input *u*, the two signatures have an empty intersection.
- X If all the distinct sets of faults are algebraic discriminable, the model is said algebraically diagnosable.

Remark

The current algebraic signature is not sufficiently discriminant!

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$$P(y, u, p, f) = m_0(y, u) + \sum_{k=1}^{q} \gamma_k(p, f) m_k(y, u) = 0 \text{ and } \begin{cases} \gamma_1(p, f) = \phi_1, \\ \vdots \\ \gamma_q(p, f) = \phi_q, \end{cases}$$

Algorithm Algebraic-Signature

✓ Groebner basis computation;

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Example:  $\ddot{x} + k(f_1 - 1)^2 x - (d + f_2)u = 0, f_1 \in [0, 2), f_2 \in [0, 2)$ with  $\phi(f) = (\phi_1, \phi_2) = (k(f_1 - 1)^2, -d - f_2).$ 

Algorithm Algebraic\_signature:  $ASig(f) = (\phi_1 - k, \phi_2 + d)$ .

#### Remarks

- $\checkmark\,$  Algebraic signature: each of its component depends only on  $\phi_{\rm k}$  and the parameters of the system;
- ✓ By construction, one of the component of the algebraic signature vanishes when at least one specific (multiple) fault occurs.

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How to certify the values of ASig?

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$$\begin{array}{rccc} ASig: & \mathbb{R}^{e} & \longrightarrow & (R[\phi_{1}, \dots, \phi_{N}])^{l} \\ & f & \mapsto & (ASig_{1}(\phi), \dots, ASig_{l}(\phi)) \,. \end{array}$$

<u>Notations</u>: ( $\mathcal{N}$  subset of  $\{1, \ldots, e\}$ )

•  $C_{p,f}$  = set of all algebraic equations and inequalities verified by p and f. <u>Example:</u>  $\ddot{x} + k(f_1 - 1)^2 x - (d + f_2)u = 0$ ,  $ASig(f) = (\phi_1 - k, \phi_2 + d)$ .  $C_{p,f} = \{0 < k < 4, 1 \le d, 0 \le f_1 < 2, 0 \le f_2 < 2\}$ . •  $S_{\mathcal{N}} = \{\gamma_1(p, f) = \phi_1, \dots, \gamma_q(p, f) = \phi_N\} \cup C_{p,f} \cup \{f_i \neq 0 | i \in \mathcal{N}\} \cup \{f_i = 0 | i \notin \mathcal{N}\}$ . <u>Example:</u>  $\ddot{x} + k(f_1 - 1)^2 x - (d + f_2)u = 0$ ,  $ASig(f) = (\phi_1 - k, \phi_2 + d)$ . If  $\mathcal{N} = \{1\}$  then  $S_{\mathcal{N}} = \{k(f_1 - 1) = \phi_1, (d + f_2) = \phi_2\} \cup C_{p,f} \cup \{f_1 \neq 0\} \cup \{f_2 = 0\}$ ; If  $\mathcal{N} = \{1, 2\}$  then  $S_{\mathcal{N}} = \{k(f_1 - 1) = \phi_1, (d + f_2) = \phi_2\} \cup C_{p,f} \cup \{f_1 \neq 0\} \cup \{f_2 \neq 0\}$ .

$$\begin{array}{rcl} \text{ASig}: & \mathbb{R}^{e} & \longrightarrow & (R[\phi_{1}, \dots, \phi_{N}])^{l} \\ & f & \mapsto & (ASig_{1}(\phi), \dots, ASig_{l}(\phi)) \, . \end{array}$$

#### Criterion

Two criterion to discriminate multiple fault signatures:

- For the multiple fault  $f_N$ ,  $S_N \cup \{ASig_k(f_N) = 0\} = \emptyset$ ?
- When  $ASig_i(f) = 0$  is equivalent to  $f_i = 0$ ?

 $\hookrightarrow$  Algorithm *ExpectedValuesOfASign*.

Example:  $\ddot{x} + k(f_1 - 1)^2 x - (d + f_2)u = 0$ ,  $ASig(f) = (\phi_1 - k, \phi_2 + d)$ .

$$C_{p,f} = \{ 0 < k < 4, 1 \le d, \\ 0 \le f_1 < 2, 0 \le f_2 < 2 \}$$

$C_{p,f}$	=	Ø

f	ASig <sub>1</sub> (f)	$ASig_2(f)$
f{}	0	0
$f_{\{1\}}$	Ø	0
f <sub>{2}</sub>	0	Ø
$f_{\{1,2\}}$	Ø	Ø

f	ASig <sub>1</sub> (f)	$ASig_2(f)$
$f_{\{\}}$	0	0
$f_{\{1\}}$		0
f <sub>{2}</sub>	0	Ø
$f_{\{1,2\}}$		Ø

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#### Conclusion

Diagnosability study:

- ✓ from the data collected on the physical system, can the chosen mathematical model permit to discriminate predefined faults that may occur on the system?
- $\checkmark$  New example of the interest of computer algebra and semialgebraic approach;
- $\checkmark\,$  Precomputations lead to efficient numerical procedures  $\rightarrow$  detect and isolate (multiple) faults.

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#### Procedure RelativeIdentifiabilityTree

**Objective:** det. the keys param. which estimations turn the model into an ident. one. **Inputs:** exhaustive summary, constraints on the parameters .

**Output:** A set of lists def. the relative identifiability tree  $\mathcal{T}$  (any prefix *b* of  $l \in \mathcal{T}$  is followed in *l* by an identifiable parameter wrt to *b* if there exists one.)

**Convention:** -p in a list *I* means that *p* is not rel. identifiable wrt the param appearing before *p* in the list *I*.



#### Branch and cut tech:

- Parameters relatively ident. wrt the same set of parameters can be permuted.
- The relative identifiability wrt a list of param. does not depend on the list of parameters but on the set they define.

#### Tutorial Diagnosability

Procedure ASign - Computation of an algebraic signature

**Objective:** obtaining of polynomials discriminating the faults and depending only on the parameters and the components of the exhaustive summary.

Inputs: exhaustive summary, single faults list.

Output: an algebraic signature.



#### Procedure ExpectedValuesOfASign

**Objective:** det. the (multiple) faults which can be discriminated with the alg. signature. **Inputs:** Alg signature, exhaustive summary, single faults list, param constraints. **Outputs:** the lists composed of a (multiple) faults and of the corresponding vector of expected values of the algebraic signature.



#### Diagnosability

#### Procedure SingleFaultCharacterization

**Objective:** Reducing the number of tests needed to determine the table of the expect. values of the algebraic signature.

Inputs: Alg. signature, exhaustive summary, single faults list, parameters contraints.

**Output:** list of 2-uplets  $[f_i, ASig_k]$  such that  $f_i \neq 0 \Leftrightarrow ASig_k \neq 0$ 



 $\rightarrow$  The output can be used as an optional argument in proc. <code>ExpectedValuesOfASign</code>.

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