Testing a model for prior identifiability

(Unit 1 of 4)

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Parameter Estimation in Physiological Models, Euro Summer School, Lipari, September 2009.

Abstract:

Before trying to estimate the parameters of a knowledge-based model from experimental data, one would like to make sure the exercise is not doomed from the start.

This unit explains how the notion of *prior identifiability* can be used for this purpose.

Methods that can be used to test linear and nonlinear knowledge-based models for prior identifiability are presented, and applied to actual biological and chemical models.

More on the material presented here can be found in

Eric Walter, *Identifiability of State Space Models*, Springer, Berlin, 1982.

Eric Walter and Luc Pronzato, *Identification of Parametric Models from Experimental Data*, Springer, London, 1997.

Introduction

(Mathematical) models may be built to:

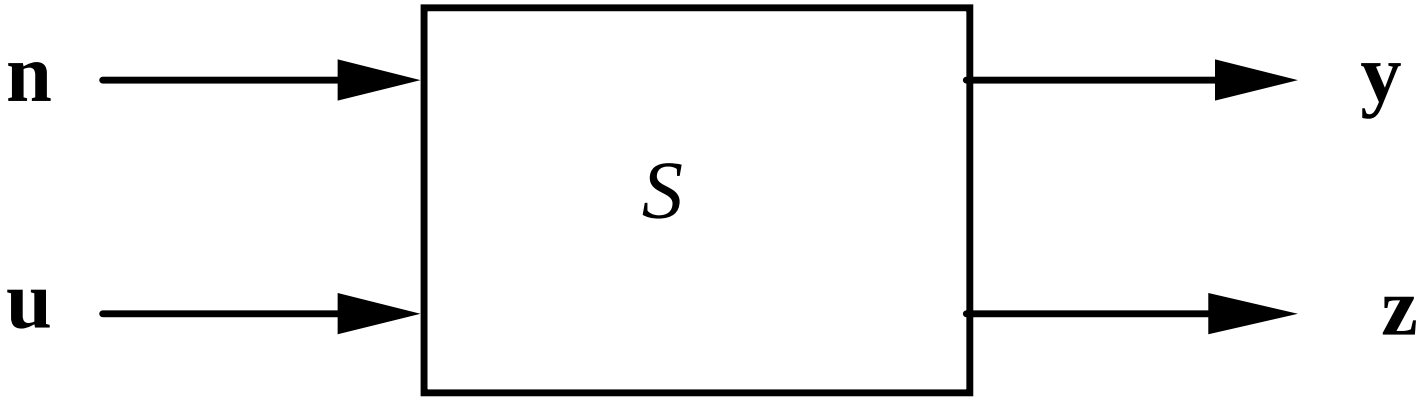
- understand,
- estimate quantities for which no sensor is available,
- test hypotheses,
- teach,
- predict behaviour,
- control processes,
- process signals
- ...

Whatever the aim, it should be made explicit (serendipity not an excuse).

System (or process)

Part of universe considered as an entity.

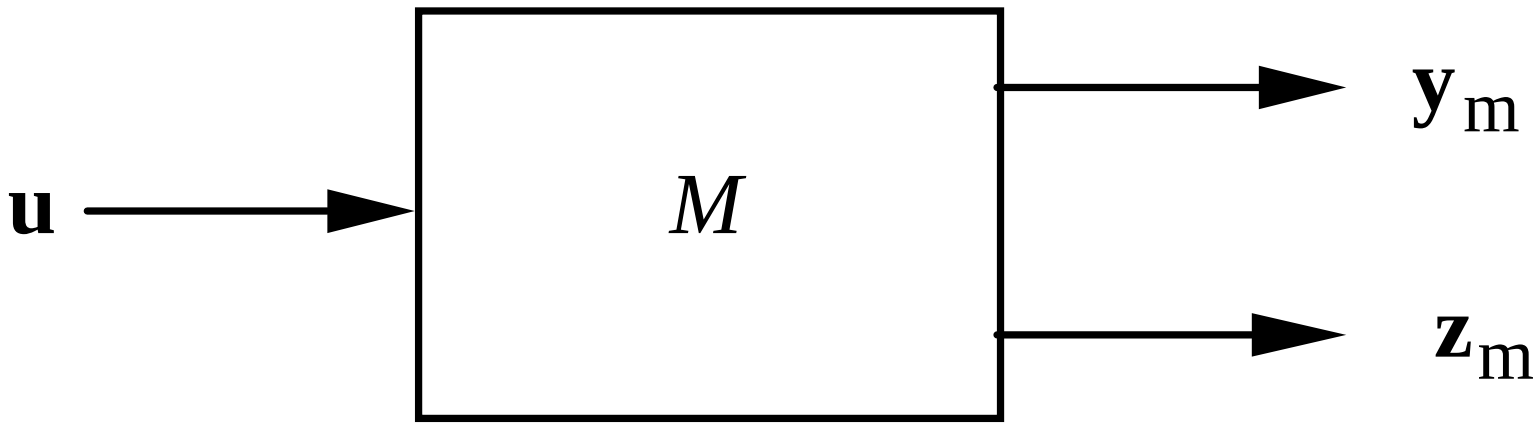
- We *observe* the *output* vector **y**.
- We *are interested in* the vector **z**, which may differ from **y**.
- We may *act on* the system by means of *inputs*, which form the vector **u**.
- We *endure* the effect of *perturbations*, or *noise* **n**.



Model

Rule to compute quantities we are interested in from what is available.

Frequently,



Model often involves unknown (constant) quantities to be estimated.

They form the parameter vector $\mathbf{p}$.

Model structure $M(\cdot) \neq$ specific model $M(\mathbf{p})$.

Once $M(\cdot)$ has been selected, $\mathbf{p}$ must be estimated, using some optimality criterion.

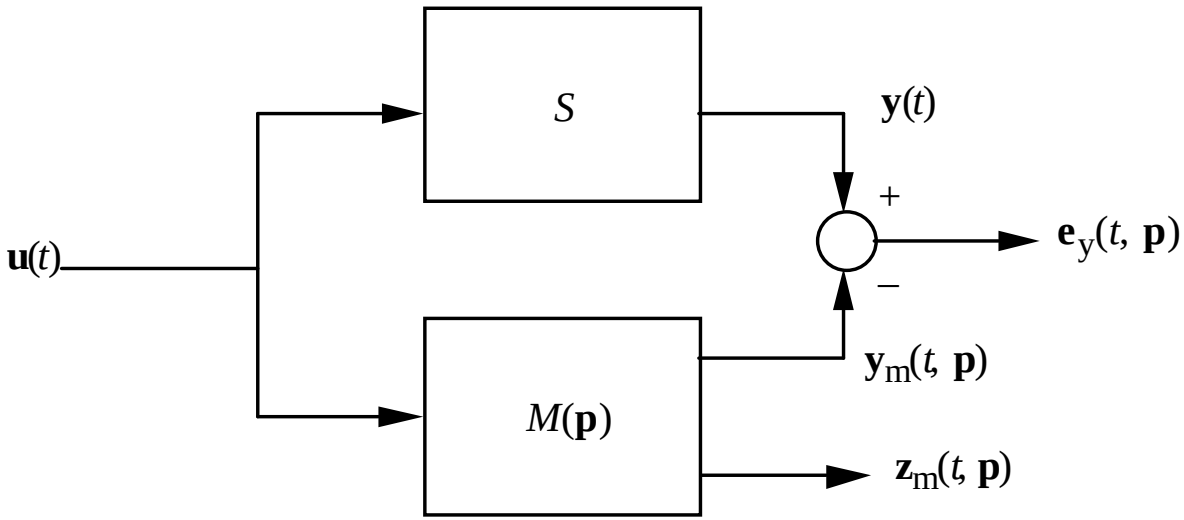
If several model structures compete for the description of the same data, their performance will also be compared with the help of a criterion.

Criterion

The *output error*

$$\mathbf{e}_{\mathrm{y}}(t, \mathbf{p}) = \mathbf{y}(t) - \mathbf{y}_{\mathrm{m}}(t, \mathbf{p})$$

should be made as small as possible, in some sense.



Scale of values needed to quantify smallness.

→ scalar function $j(\cdot)$ of the parameters and possibly of the structure, called the *cost function*.

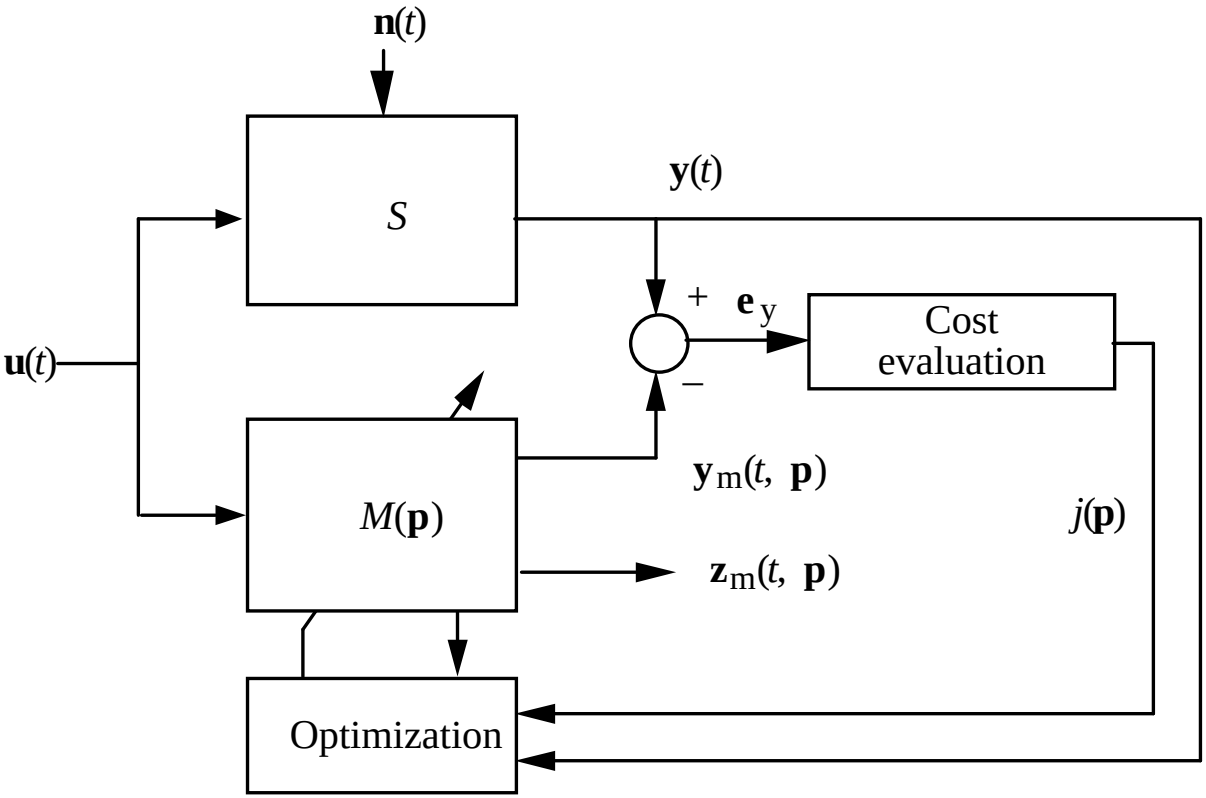
Example:

$$j(\mathbf{p}) = \sum_{\text{measurement times}} \sum_{\text{output components}} \text{square of error}(\mathbf{p})$$

Cost must be optimized with respect to **p**.

Optimization

A possible scheme (out of many) is



Before attempting the operation, we wish to make sure it is not doomed from the start.

Notion of prior identifiability will provide a partial answer.

Let us first distinguish

- knowledge-based and behavioural models (schematic and simplistic but useful),
- linear and nonlinear models (very important).

Knowledge-based and behavioural models

Knowledge-based models built from basic principles, by writing down balance equations.

Consider, for instance, the chemical reaction

$$\mathrm{A} \underset{p_2}{\overset{p_1}{\rightleftharpoons}} \mathrm{B} \xrightarrow{p_3} \mathrm{C}$$

If reactions obey first-order kinetics and reactor isothermal and well stirred, then

$$\frac{\mathrm{d}[A]}{\mathrm{d}t} = -p1[A] + p2[B],$$
$$\frac{\mathrm{d}[B]}{\mathrm{d}t} = p1[A] - (p2 + p3)[B],$$
$$\frac{\mathrm{d}[C]}{\mathrm{d}t} = p3[B].$$

Model structure thus imposed by the prior knowledge (or hypotheses) about the system.

Parameters p_i are kinetic constants.

State variables [A], [B] and [C] are concentrations.

Parameters and state variables of knowledge-based models have a precise concrete meaning, so we usually wish to get accurate estimates of them.

At the other hand of the spectrum, we have:

Behavioural models, which merely approximate observed behaviour.

Now prior knowledge required.

Not even necessary to know what the inputs and outputs stand for.

The parameters of behavioural models usually have no physical meaning.

For example, polynomial model

$$y_{\mathrm{m}}(t, \mathbf{p}) = p_1 + p_2 t + p_3 t^2 + p_4 t^3 + \ldots$$

can reproduce, with arbitrary precision, any finite set of experimental data

$$y(t_i),\ i = 1, \ldots, n_{\mathrm{t}},$$

provided that polynomial degree large enough.

Particularly simplistic example of a behavioural model.

Behavioural models are in general simpler to simulate and more suited to control than knowledge-based models (easy to find counter examples, though).

We shall be concerned here with knowledge-based models.

Linear and nonlinear models

Two types of linearity must be distinguished.

$\mathbf{y}_m(t, \mathbf{p}, \mathbf{u}) \triangleq$ output at time t of $M(\mathbf{p})$ when input $\mathbf{u}(\tau)$, $0 \leq \tau \leq t$, has been applied from zero initial condition.

$M(\cdot)$ is *linear in its inputs (LI)* if $\mathbf{y}_m$ satisfies superposition principle with respect to $\mathbf{u}$:

$$\forall\ (\lambda, \mu) \in \mathbb{R}^2,\ \forall\ t \in \mathbb{R}^+,\ \mathbf{y}_m(t, \mathbf{p}, \lambda\mathbf{u}_1 + \mu\mathbf{u}_2) = \lambda\mathbf{y}_m(t, \mathbf{p}, \mathbf{u}_1) + \mu\mathbf{y}_m(t, \mathbf{p}, \mathbf{u}_2).$$

When control engineers speak of linear models, they usually refer to this type of linearity.

Moreover, they often assume implicitly that the model is time-invariant, *i.e.*, that its behaviour is invariant under a translation of the origin of time.

LI models are a (sometime very useful) approximations.

$M(\cdot)$ is *linear in its parameters (LP)* if $\mathbf{y}_\mathrm{m}$ satisfies superposition principle with respect to $\mathbf{p}$:

$$\forall\ (\lambda, \mu) \in \mathbb{R}^2, \forall\ t \in \mathbb{R}^+, \mathbf{y}_\mathrm{m}(t, \lambda\mathbf{p}_1 + \mu\mathbf{p}_2, \mathbf{u}) = \lambda\mathbf{y}_\mathrm{m}(t, \mathbf{p}_1, \mathbf{u}) + \mu\mathbf{y}_\mathrm{m}(t, \mathbf{p}_2, \mathbf{u}).$$

When statisticians speak of linear models, they usually refer to this type of linearity.

Extremely useful to know whether the model structure considered is LP or not, and LI or not

$\frac{\mathrm{d}y_\mathrm{m}}{\mathrm{d}t} = -p_1 y_\mathrm{m} + p_2 u$ is LI but not LP.

Very many knowledge-based models are not LP!

Structural properties of models

Once $M(\cdot)$ chosen, we wish to study its properties independently of the value taken by $\mathbf{p}$.

This could allow problem detection even before data collection.

A property is *structural* (or *generic*) if it is true for *almost any* value of $\mathbf{p}$.

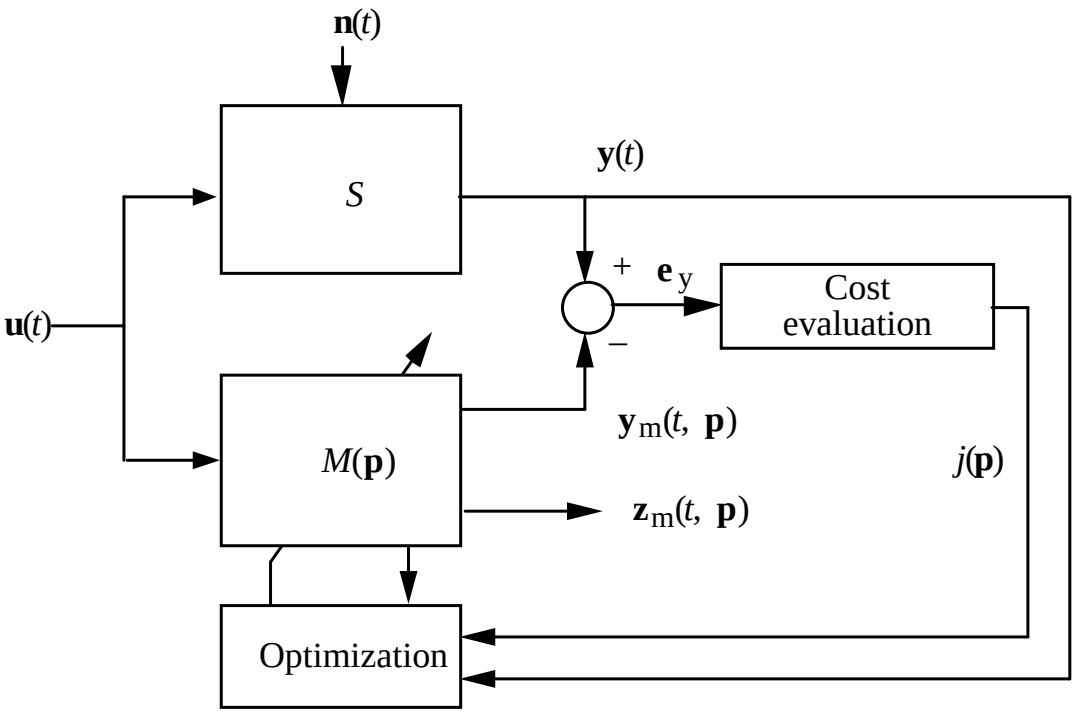
Thus, the probability of randomly picking an atypical value of $\mathbf{p}$ is zero.

Two structural properties are of special importance for us:

- *identifiability*
- *distinguishability*.

Identifiability

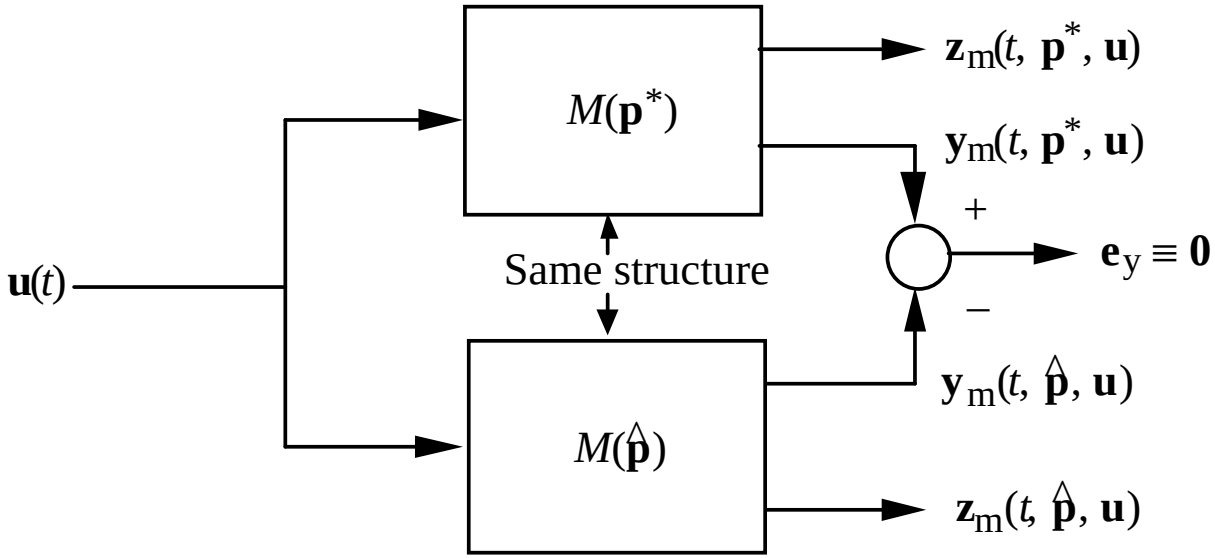
Can we hope to estimate a meaningful $\hat{\mathbf{p}}$?



Such a vague question has no answer, so we consider an idealized framework, where

- process and model have the same structure,
- data are noise-free,
- input **u** and measurement times can be chosen at will.

Always possible then to tune $\hat{\mathbf{p}}$ so as to make the model input-output behaviour identical to that of the process, which we denote by $M(\mathbf{p}^*) = M(\hat{\mathbf{p}})$.



We wish to know whether $M(\mathbf{p}^*) = M(\hat{\mathbf{p}})$ implies $\hat{\mathbf{p}} = \mathbf{p}^*$.

More precisely,

- Parameter p_i is *structurally globally* (or *uniquely*) *identifiable* (*s.g.i.*) if for almost any $\mathbf{p}^*$ in $\mathbb{P}$,

$$M(\hat{\mathbf{p}}) = M(\mathbf{p}^*) \Rightarrow \hat{p}_i = p_i^* .$$

- Structure $M(\cdot)$ is s.g.i. if all its parameters are s.g.i.

When one cannot prove that $M(.)$ is s.g.i., one may try to establish that it is at least locally identifiable.

- Parameter p_i is *structurally locally identifiable (s.l.i.)* if for almost any $\mathbf{p}^*$ in $\mathbb{P}$, there exists a neighbourhood $\mathbb{V}(\mathbf{p}^*)$ such that

$$\hat{\mathbf{p}} \in \mathbb{V}(\mathbf{p}^*) \text{ and } M(\hat{\mathbf{p}}) = M(\mathbf{p}^*) \Rightarrow \hat{p}_i = p_i^* .$$

[Local identifiability thus necessary for global identifiability.]

- Structure $M(\cdot)$ is s.l.i. if all its parameters are s.l.i.

- Parameter p_i is *structurally unidentifiable (s.u.i.)* if for almost any $\mathbf{p}^*$ in $\mathbb{P}$, there is no neighbourhood $\mathbb{V}(\mathbf{p}^*)$ such that

$$\hat{\mathbf{p}} \in \mathbb{V}(\mathbf{p}^*) \text{ and } M(\hat{\mathbf{p}}) = M(\mathbf{p}^*) \Rightarrow \hat{p}_i = p_i^*$$

- Structure $M(\cdot)$ is s.u.i. if one at least of its parameters is s.u.i.

Dumb example:

Let V be the difference of potential between the extremities of a resistor (input), and I be the resulting current through the resistor (output). With Ohm's model

$$U = R \cdot I$$

parameter R is s.g.i.

If Ohm had been stupid enough to choose

$$U = (\cos R) \cdot I$$

then R would be s.l.i. With

$$U = R_1 \cdot R_2 \cdot I$$

R_1 and R_1 would be s.u.i.

REMARKS

- Some parameters of an s.u.i. model may be s.l.i. or even s.g.i.
- Identifiability may depend on the numerical value taken by $\mathbf{p}$ without the atypical region being of zero measure. Impossible then to reach a structural conclusion.
- If the input and measurement times are fixed *a priori*, it suffices to replace $M(\hat{\mathbf{p}}) = M(\mathbf{p}^*)$ in the definitions by $\mathbf{y}^{\mathrm{m}}(\hat{\mathbf{p}}) = \mathbf{y}^{\mathrm{m}}(\mathbf{p}^*)$, where $\mathbf{y}^{\mathrm{m}}(\mathbf{p})$ stands for the vector obtained by concatenating all available output vectors $\mathbf{y}_{\mathrm{m}}(t_i, \mathbf{p}, \mathbf{u})$, $i = 1, \ldots, n_{\mathrm{t}}$.

Many methods available for testing models for structural identifiability.

We shall only consider non-LP models (identifiability of LP models is a trivial matter), and start by methods for (time-invariant) LI models.

Consider a structure $M(\cdot)$ described by

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathbf{x} = \mathbf{A}(\mathbf{p})\mathbf{x} + \mathbf{B}(\mathbf{p})\mathbf{u}\,,\;\; \mathbf{x}(0) = \mathbf{x}_0(\mathbf{p}),$$

$$\mathbf{y}_\mathrm{m} = \mathbf{C}(\mathbf{p})\mathbf{x} + \mathbf{D}(\mathbf{p})\mathbf{u}.$$

(LI, not LP)

Laplace-transform approach

Eliminating state $\mathbf{x}$ from Laplace transform of previous equations, we get

$$\mathbf{y}_\mathrm{m}(s, \mathbf{p}) = \mathbf{H}_1(s, \mathbf{p})\mathbf{u}(s) + \mathbf{H}_2(s, \mathbf{p})\mathbf{x}_0(\mathbf{p}),$$

with

$$\mathbf{H}_1(s, \mathbf{p}) = \mathbf{C}(\mathbf{p})[s\mathbf{I} - \mathbf{A}(\mathbf{p})]^{-1}\mathbf{B}(\mathbf{p}) + \mathbf{D}(\mathbf{p}) \text{ and } \mathbf{H}_2(s, \mathbf{p}) = \mathbf{C}(\mathbf{p})[s\mathbf{I} - \mathbf{A}(\mathbf{p})]^{-1}.$$

$$M(\hat{\mathbf{p}}) = M(\mathbf{p}^*) \Leftrightarrow \mathbf{y}_m(s, \hat{\mathbf{p}}) - \mathbf{y}_m(s, \mathbf{p}^*) \equiv \mathbf{0} \quad \forall\, s, \mathbf{u}(s).$$

→ set of algebraic equations binding $\hat{\mathbf{p}}$ and $\mathbf{p}^*$.

If for almost any $\mathbf{p}^*$

- solution for $\hat{\mathbf{p}}$ is unique, then $M(\cdot)$ s.g.i.
- set of solutions for $\hat{\mathbf{p}}$ is finite or denumerable, then $M(\cdot)$ s.l.i.
- set of solutions for $\hat{\mathbf{p}}$ is not denumerable, then $M(\cdot)$ s.u.i.

Any parameter that takes the same value in all solutions is s.g.i.

Any parameter that takes its values in a finite or denumerable set is s.l.i.

Writing $\mathbf{H}_1$ and $\mathbf{H}_2$ in *canonical form* simplifies computation considerably.

Then

$M(\hat{\mathbf{p}}) = M(\mathbf{p}^*) \Leftrightarrow$ the *coefficients* of $\mathbf{H}_1$ and $\mathbf{H}_2$ have the same value for $\mathbf{p} = \hat{\mathbf{p}}$ and $\mathbf{p} = \mathbf{p}^*$.

Canonical form for instance obtained by

- writing each entry of the transfer matrix as a ratio of polynomials ordered in s,
- simplifying numerator and denominator by GCD (only the controllable and observable part of the model remains),
- setting the coefficient of the denominator monomial with highest (or lowest) degree in s equal to one.

EXAMPLE

Consider the (LI, non-LP) compartmental model structure defined by

$$\frac{\mathrm{d}}{\mathrm{d}t}\, x_1 = -(p_1 + p_2)x_1 + p_3 x_2 + u, \qquad x_1(0) = 0,$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\, x_2 = p_1 x_1 - p_3 x_2, \qquad x_2(0) = 0,$$
$$y_\mathrm{m} = x_2.$$

Take Laplace transform

$$(s + p_1 + p_2)x_1(s) = p_3 x_2(s) + u(s),$$

$$(s + p_3)x_2(s) = p_1 x_1(s),$$

$$y_\mathrm{m}(s) = x_2(s).$$

Eliminate x_1 and x_2 to get

$$(s + p_1 + p_2)(s + p_3)y_{\mathrm{m}}(s) = p_1 p_3 y_{\mathrm{m}}(s) + p_1 u(s).$$

Transfer function (in canonical form) is

$$H_1(s, \mathbf{p}) = \frac{p1}{s^2 + s(p1 + p2 + p3) + p2p3} \quad .$$

$M(\hat{\mathbf{p}}) = M(\mathbf{p}^*)$ therefore equivalent to

$$\hat{p}1 = p1^* ,$$
$$\hat{p}2 + \hat{p}3 = p2^* + p3^* ,$$
$$\hat{p}2\hat{p}3 = p2^* p3^* .$$

Now

$$\hat{p}_1 = p_1^* ,$$
$$\hat{p}_2 + \hat{p}_3 = p_2^* + p_3^* ,$$
$$\hat{p}_2 \hat{p}_3 = p_2^* p_3^* ,$$

has two solutions for $\hat{\mathbf{p}}$, namely

$$\hat{\mathbf{p}}_1 = (p_1^* , p_2^* , p_3^*)^T \quad \text{and} \quad \hat{\mathbf{p}}_2 = (p_1^* , p_3^* , p_2^*)^T.$$

First parameter, which takes the same value in the two solutions, is s.g.i.

The other two, which each can take two values, are only s.l.i.

From noise-free data, possible to compute the true value for p_1, whereas two possible values will be obtained for p_2 and p_3.

REMARKS

- With an iterative local optimization algorithm, we would (at best) have found either of the two solutions. We can now generate the other.
- If $\mathbf{p}^*$ such that $p_1 = 0$, then output is identically zero whatever the input, so p_2 and p_3 become unidentifiable. These parameters are nevertheless s.l.i., for $p_1 = 0$ is atypical.
- Since model not s.g.i., impossible to reconstruct state uniquely from the knowledge of input-output behaviour. Depending on the model selected, two possible values for x_1 will be obtained.
- More generally, if the vector $\mathbf{z}$ of the quantities of interest depends on state variables that are not measured, important to make sure that model is s.g.i., or at least that

$$M(\hat{\mathbf{p}}) = M(\mathbf{p}^*) \Rightarrow \mathbf{z}_{\mathrm{m}}(t, \hat{\mathbf{p}}, \mathbf{u}) \equiv \mathbf{z}_{\mathrm{m}}(t, \mathbf{p}^*, \mathbf{u}).$$

- The existence of a true value of the parameters need not be assumed; $\mathbf{p}^*$ may be the parameter vector of a model generating a satisfactory input-output behaviour.

Note: If model only to be used for prediction or control of process *output*, with no constraint on quantities that cannot be measured directly, then identifiability is not an issue.

Similarity transformation approach

Assume "process" $M(\mathbf{p}^*)$ described by

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathbf{x}^* = \mathbf{A}(\mathbf{p}^*)\mathbf{x}^* + \mathbf{B}(\mathbf{p}^*)\mathbf{u},\;\; \mathbf{x}^*(0) = \mathbf{x}_0(\mathbf{p}^*),$$

$$\mathbf{y}_\mathrm{m} = \mathbf{C}(\mathbf{p}^*)\mathbf{x}^* + \mathbf{D}(\mathbf{p}^*)\mathbf{u}.$$

Let $\hat{\mathbf{x}} = \mathbf{T}\mathbf{x}^*$, with $\mathbf{T}$ invertible. Then

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\hat{\mathbf{x}} = \mathbf{T}\mathbf{A}(\mathbf{p}^*)\mathbf{T}^{-1}\hat{\mathbf{x}} + \mathbf{T}\mathbf{B}(\mathbf{p}^*)\mathbf{u},\;\; \hat{\mathbf{x}}(0) = \mathbf{T}\mathbf{x}_0(\mathbf{p}^*),$$

$$\mathbf{y}_\mathrm{m} = \mathbf{C}(\mathbf{p}^*)\mathbf{T}^{-1}\hat{\mathbf{x}} + \mathbf{D}(\mathbf{p}^*)\mathbf{u},$$

will have the same input-output behaviour as $M(\mathbf{p}^*)$. It will correspond to an $M(\hat{\mathbf{p}})$ if and only if

$$\begin{cases} \mathbf{A}(\hat{\mathbf{p}}) = \mathbf{T}\mathbf{A}(\mathbf{p}^*)\mathbf{T}^{-1}, \\ \mathbf{B}(\hat{\mathbf{p}}) = \mathbf{T}\mathbf{B}(\mathbf{p}^*), \\ \mathbf{C}(\hat{\mathbf{p}}) = \mathbf{C}(\mathbf{p}^*)\mathbf{T}^{-1}, \\ \mathbf{D}(\hat{\mathbf{p}}) = \mathbf{D}(\mathbf{p}^*), \\ \mathbf{x}_0(\hat{\mathbf{p}}) = \mathbf{T}\mathbf{x}_0(\mathbf{p}^*), \end{cases}$$

which is a *sufficient* set of conditions for $M(\hat{\mathbf{p}}) = M(\mathbf{p}^*)$. It turns out to be also *necessary*, provided that $M(\mathbf{p}^*)$ be observable and controllable (assumed here).

Structural identifiability of $M(\cdot)$ can then be tested by looking for all solutions for $(\hat{\mathbf{p}}, \mathbf{T})$.

If for almost any $\mathbf{p}^*$

- only solution is $(\hat{\mathbf{p}}, \mathbf{T}) = (\mathbf{p}^*, \mathbf{I})$, then $M(\cdot)$ is s.g.i.
- set of solutions for $\hat{\mathbf{p}}$ is finite or denumerable, then $M(\cdot)$ is s.l.i.

EXAMPLE (CONTINUED)

State and observation equations are such that

$$\mathbf{A}(\mathbf{p}) = \begin{bmatrix} -(p1 + p2) & p3 \\ p1 & -p3 \end{bmatrix}, \quad \mathbf{B}(\mathbf{p}) = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \mathbf{x}(0) = \mathbf{0},$$

$$\mathbf{C}(\mathbf{p}) = \begin{bmatrix} 0 & 1 \end{bmatrix}, \quad \mathbf{D}(\mathbf{p}) = \mathbf{0}.$$

$M(\cdot)$ structurally controllable and observable, so similarity transformation approach applies.

Zero initial conditions bring no information on $\mathbf{T}$.

Exploit first the structures of $\mathbf{B}$ and $\mathbf{C}$, with $t_{ik} = [\mathbf{T}]_{ik}$:

$$\mathbf{C}(\hat{\mathbf{p}})\mathbf{T} = \mathbf{C}(\mathbf{p}^*) \Longrightarrow t_{21} = 0,\ t_{22} = 1,$$
$$\mathbf{B}(\hat{\mathbf{p}}) = \mathbf{T}\mathbf{B}(\mathbf{p}^*) \Rightarrow t_{11} = 1.$$

So

$$\mathbf{T}(\alpha) = \begin{bmatrix} 1 & \alpha \\ 0 & 1 \end{bmatrix}.$$

The set of all possible matrices **A** satisfies

$$\mathbf{A}(\hat{\mathbf{p}}) = \mathbf{T}(\alpha)\mathbf{A}(\mathbf{p}^*)\mathbf{T}^{-1}(\alpha) = \begin{bmatrix} -(p_1^* + p_2^*) + \alpha p_1^* & \alpha(p_1^* + p_2^*) + p_3^* - \alpha^2 p_1^* - \alpha p_3^* \\ p_1^* & -\alpha p_1^* - p_3^* \end{bmatrix}.$$

In $\mathbf{A}(\hat{\mathbf{p}})$, the sum of the terms of the second column must be equal to zero, so

$$\alpha^2 p_1^* + \alpha(p_3^* - p_2^*) = 0.$$

This equation has two solutions for α, namely

$$\alpha = 0 \quad \text{and} \quad \alpha = \frac{p_2^* - p_3^*}{p_1^*}.$$

$$\alpha = 0 \quad \Rightarrow \quad \mathbf{T} = \mathbf{I},\ \hat{\mathbf{p}} = \mathbf{p}^* \text{ and } \alpha = \frac{p_2^* - p_3^*}{p_1^*} \quad \Longrightarrow \quad \mathbf{T} \neq \mathbf{I},\ \hat{\mathbf{p}} = \begin{bmatrix} p_1^* \\ p_3^* \\ p_2^* \end{bmatrix}.$$

Same conclusion as with Laplace-transform approach: $M(\cdot)$ is s.l.i.; only p_1 is s.g.i., p_2 and p_3 can be exchanged without modifying the input-output behaviour.

Even from noise-free data, impossible to estimate $\mathbf{p}^*$ and $\mathbf{x}^*$ uniquely, but all their possible values can now be computed.

REMARK

Although conclusion does not depend on method, the required computations do.

Depending on the example considered, one or the other approach may turn out to be *much* simpler.

The methods to be considered now also apply to non-LI models.

Taylor series approach

Assume $M(\cdot)$ described by

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathbf{x}(t) = \mathbf{f}[\mathbf{x}(t), \mathbf{u}(t), t, \mathbf{p}], \quad \mathbf{x}(0) = \mathbf{x}_0(\mathbf{p}), \quad \mathbf{y}_\mathrm{m}(t, \mathbf{p}) = \mathbf{h}[\mathbf{x}(t), \mathbf{p}],$$

where **f** and **h** are infinitely continuously differentiable.

Let

$$\mathbf{a}_k(\mathbf{p}) = \lim_{t\to 0+} \frac{\mathrm{d}^k}{\mathrm{d}t^k}\,\mathbf{y}_\mathrm{m}(t, \mathbf{p}).$$

$$M(\hat{\mathbf{p}}) = M(\mathbf{p}^*) \Longrightarrow \mathbf{a}_k(\hat{\mathbf{p}}) = \mathbf{a}_k(\mathbf{p}^*), \quad k = 0, 1, \ldots$$

A *sufficient* condition for $M(\cdot)$ to be s.g.i. is therefore

$$\mathbf{a}_k(\hat{\mathbf{p}}) = \mathbf{a}_k(\mathbf{p}^*),\ k = 0, 1, \ldots, k_{\max}, \quad \Rightarrow \quad \hat{\mathbf{p}} = \mathbf{p}^*,$$

with $k_{\max}$ small enough for the computation to remain tractable.

EXAMPLE

Consider the matrix of all impulse responses of a LI state-space model (with $\mathbf{D} = \mathbf{0}$)

$$\mathbf{Y}_{\mathrm{m}}(t, \mathbf{p}) = \mathbf{C}(\mathbf{p})\exp[\mathbf{A}(\mathbf{p})t]\mathbf{B}(\mathbf{p}).$$

Since

$$\lim_{t\to 0+} \frac{\mathrm{d}^k}{\mathrm{d}t^k}\, \mathbf{Y}_{\mathrm{m}}(t, \mathbf{p}) = \mathbf{C}(\mathbf{p})\mathbf{A}^k(\mathbf{p})\mathbf{B}(\mathbf{p}),$$

the Taylor series approach amounts to testing identifiability from identity of the *Markov parameters*

$$\mathbf{C}(\hat{\mathbf{p}})\mathbf{A}^k(\hat{\mathbf{p}})\mathbf{B}(\hat{\mathbf{p}}) = \mathbf{C}(\mathbf{p}^*)\mathbf{A}^k(\mathbf{p}^*)\mathbf{B}(\mathbf{p}^*),\ k = 0, 1, \ldots, k_{\max},$$

a method that usually turns out to be more complicated than the Laplace transform and similarity transformation approaches.

EXAMPLE

Consider now the unforced non-LI structure $M(\cdot)$ defined by

$$\frac{\mathrm{d}}{\mathrm{d}t}\ \mathbf{x} = \begin{bmatrix} -p_1x_1 - p_2(1 - p_3x_2)x_1 \\ p_2(1 - p_3x_2)x_1 - p_4x_2 \end{bmatrix}, \quad \mathbf{x}(0) = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, y_{\mathrm{m}}(t, \mathbf{p}) = x_1.$$

Successive derivatives of y_m at $t = 0^+$ satisfy

$$a_0(\mathbf{p}) = 1,$$
$$a_1(\mathbf{p}) = -(p_1 + p_2),$$
$$a_2(\mathbf{p}) = (p_1 + p_2)^2 + p_2^2\, p_3,$$
$$a_3(\mathbf{p}) = -p_2^3\, p_3^2 - 4\, p_2^2\, p_3(p_1 + p_2) - p_2^2\, p_3 p_4 - (p_1 + p_2)^3,$$
$$\ldots$$

and

$$\mathbf{a}_k(\hat{\mathbf{p}}) = \mathbf{a}_k(\mathbf{p}^*),\ \ k = 1, 2, \ldots, 5, \ \Longrightarrow\ \hat{\mathbf{p}} = \mathbf{p}^*.$$

$M(\cdot)$ is therefore s.g.i.

REMARK

If p_3 is set to zero, the model becomes LI and s.u.i. (LI models tend to be less identifiable than their non-LI counterparts!)

Local state isomorphism approach

Extends similarity transformation approach to non-LI models.

Assume $M(\cdot)$ defined by

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathbf{x}(t) = \mathbf{f}[\mathbf{x}(t), \mathbf{p}] + u(t)\mathbf{g}[\mathbf{x}(t), \mathbf{p}], \qquad \mathbf{x}(0) = \mathbf{x}_0(\mathbf{p}), \qquad \mathbf{y}_{\mathrm{m}}(t, \mathbf{p}) = \mathbf{h}[\mathbf{x}(t), \mathbf{p}],$$

where $\mathbf{f}$, $\mathbf{g}$ and $\mathbf{h}$ are analytic, u is a measurable bounded function and $M(\mathbf{p})$ is locally reduced at $\mathbf{x}_0(\mathbf{p})$ for almost any $\mathbf{p}$ (which corresponds to a notion of observability and controllability).

Let $\mathbf{x}^*$ be the state of $M(\mathbf{p}^*)$ and $\hat{\mathbf{x}}$ that of $M(\hat{\mathbf{p}})$.

$M(\mathbf{p}^*)$ and $M(\hat{\mathbf{p}})$ will have the same input-output behaviour for any u up to some $t_1 > 0$ if and only if there exists a local state isomorphism: $\mathbb{V}_0^* \to \mathbb{R}^n$, $\mathbf{x}^* \to \hat{\mathbf{x}} = \boldsymbol{\phi}(\mathbf{x}^*)$ such that

for any $\mathbf{x}^*$ in the neighbourhood $\mathbb{V}_0^*$ of $\mathbf{x}_0(\mathbf{p}^*)$

ϕ is a diffeomorphism: $$\text{rank}\,\frac{\partial\phi(\mathbf{x})}{\partial\mathbf{x}^T}\Big|_{\mathbf{x}=\mathbf{x}^*} = n, \qquad \text{(i)}$$

initial states correspond: $$\phi(\mathbf{x}_0^*) = \hat{\mathbf{x}}_0, \qquad \text{(ii)}$$

drift terms correspond: $$\mathbf{f}(\hat{\mathbf{x}}, \hat{\mathbf{p}}) = \mathbf{f}[\phi(\mathbf{x}^*), \hat{\mathbf{p}}] = \frac{\partial\phi(\mathbf{x})}{\partial\mathbf{x}^T}\Big|_{\mathbf{x}=\mathbf{x}^*} \mathbf{f}(\mathbf{x}^*, \mathbf{p}^*), \qquad \text{(iii)}$$

control terms correspond: $$\mathbf{g}(\hat{\mathbf{x}}, \hat{\mathbf{p}}) = \mathbf{g}[\phi(\mathbf{x}^*), \hat{\mathbf{p}}] = \frac{\partial\phi(\mathbf{x})}{\partial\mathbf{x}^T}\Big|_{\mathbf{x}=\mathbf{x}^*} \mathbf{g}(\mathbf{x}^*, \mathbf{p}^*), \qquad \text{(iv)}$$

observations correspond: $$\mathbf{h}(\hat{\mathbf{x}}, \hat{\mathbf{p}}) = \mathbf{h}[\phi(\mathbf{x}^*), \hat{\mathbf{p}}] = \mathbf{h}(\mathbf{x}^*, \mathbf{p}^*). \qquad \text{(v)}$$

After checking that $M(\mathbf{p})$ is locally reduced at $\mathbf{x}_0(\mathbf{p})$, one can look for all solutions for $\hat{\mathbf{p}}$ and ϕ of (i) – (v).

If for almost any $\mathbf{p}^*$ the only possible solution is $\hat{\mathbf{p}} = \mathbf{p}^*$ and $\phi(\mathbf{x}^*) = \mathbf{x}^*$, then M is s.g.i.

May involve fairly complicated computation first to check that $M(\mathbf{p})$ is locally reduced and then to solve (i) – (v) for $\hat{\mathbf{p}}$ and ϕ.

But

If there exists $\mathbf{p}_0$ such that $M(\mathbf{p}_0)$ is LI, controllable and observable, then $M(\cdot)$ is locally reduced at $\mathbf{x}(0) = \mathbf{0}$.

If

- the components of $\mathbf{f}$ and $\mathbf{g}$ are polynomials in $\mathbf{x}$ parametrized by $\mathbf{p}$
- and $\mathbf{h}[\mathbf{x}(t, \mathbf{p}), \mathbf{p}] = \mathbf{C}(\mathbf{p})\mathbf{x}(t, \mathbf{p})$,

then ϕ is a linear transformation $\hat{\mathbf{x}} = \mathbf{T}\mathbf{x}^*$, which drastically simplifies calculations.

Conditions (i) – (v) then become

$$\det \mathbf{T} \neq 0, \qquad \text{(i')}$$

$$\mathbf{T}\mathbf{x}_0(\mathbf{p}^*) = \mathbf{x}_0(\hat{\mathbf{p}}), \qquad \text{(ii')}$$

$$\mathbf{f}(\mathbf{T}\mathbf{x}^*, \hat{\mathbf{p}}) = \mathbf{T}\mathbf{f}(\mathbf{x}^*, \mathbf{p}^*), \qquad \text{(iii')}$$

$$\mathbf{g}(\mathbf{T}\mathbf{x}^*, \hat{\mathbf{p}}) = \mathbf{T}\mathbf{g}(\mathbf{x}^*, \mathbf{p}^*), \qquad \text{(iv')}$$

$$\mathbf{C}(\hat{\mathbf{p}})\mathbf{T} = \mathbf{C}(\mathbf{p}^*). \qquad \text{(v')}$$

For LI models also, the local isomorphism is a linear transformation, and the method reduces to the similarity transformation approach.

EXAMPLE

Consider the non-LI structure $M(\cdot)$ defined by

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathbf{x} = \begin{bmatrix} -p_1x_1 - p_2(1 - p_3x_2)x_1 \\ p_2(1 - p_3x_2)x_1 - p_4x_2 \end{bmatrix} + \begin{bmatrix} 1 \\ 0 \end{bmatrix} u, \quad \mathbf{x}(0) = \mathbf{0}, \quad y_{\mathrm{m}}(t, \mathbf{p}) = x_2 = \begin{bmatrix} 0 & 1 \end{bmatrix} \mathbf{x}.$$

Trivial to check that when $p_3 = 0$ the structure becomes LI and structurally controllable and observable, so M is structurally locally reduced and the local state isomorphism approach applies.

$M(\cdot)$ is polynomial, so $\boldsymbol{\phi}(\mathbf{x}) = \mathbf{T}\mathbf{x}$, and Conditions (i') – (v') express that $M(\mathbf{p}^*) = M(\hat{\mathbf{p}})$.

Condition (ii') brings no information on $\mathbf{T}$. Conditions (iv') and (v') imply that $\mathbf{T}$ can be written as

$$\mathbf{T}(\alpha) = \begin{bmatrix} 1 & \alpha \\ 0 & 1 \end{bmatrix}.$$

Condition (iii') then translates into

$$\mathbf{f}(\mathbf{T}\mathbf{x}^*, \hat{\mathbf{p}}) = \begin{bmatrix} -\hat{p}_1(x_1^* + \alpha x_2^*) - \hat{p}_2(1 - \hat{p}_3 x_2^*)(x_1^* + \alpha x_2^*) \\ \hat{p}_2(1 - \hat{p}_3 x_2^*)(x_1^* + \alpha x_2^*) - \hat{p}_4 x_2^* \end{bmatrix}$$

$$= \mathbf{T}\mathbf{f}(\mathbf{x}^*, \mathbf{p}^*) = \begin{bmatrix} 1 & \alpha \\ 0 & 1 \end{bmatrix} \begin{bmatrix} -p_1^* x_1^* - p_2^*(1 - p_3^* x_2^*) x_1^* \\ p_2^*(1 - p_3^* x_2^*) x_1^* - p_4^* x_2^* \end{bmatrix}.$$

Second row equivalent to

$$-\alpha \hat{p}_2 \hat{p}_3 x_2^{*\,2} + (p_2^* p_3^* - \hat{p}_2 \hat{p}_3) x_1^* x_2^* + (\hat{p}_2 - p_2^*) x_1^* + (p_4^* + \alpha \hat{p}_2 - \hat{p}_4) x_2^* = 0.$$

Must hold true for *any* $\mathbf{x}^*$ around $\mathbf{0}$ and almost any $\mathbf{p}^*$, so $\hat{p}_2 = p_2^*$, $\hat{p}_3 = p_3^*$, $\alpha = 0$ and $\hat{p}_4 = p_4^*$.

Processing first row in the same manner proves that $\hat{p}_1 = p_1^*$, so $M(\cdot)$ s.g.i.

Use of elimination theory

Computer-algebra software such as MAPLE can be used to

- get equations expressing $M(\hat{\mathbf{p}}) = M(\mathbf{p}^*)$
- solve them.

Equations can often be put into the form of sets of polynomial equations in several unknowns, which can be transformed into triangular ones with the help of elimination theory.

These sets of triangular equations can then be solved by considering a sequence of single-variable polynomials.

Since $\mathbf{p}$ is assumed to belong to $\mathbb{R}^{n_p}$, one should only consider real solutions, which may complicate the matter.

Differential algebra, in which differentiation is added to the classical axioms of algebra, makes it possible to use a similar approach to eliminate state variables.

When differential input-output relations can thus be obtained, they can be used to study identifiability.

EXAMPLE

Volmer-Heyrovski mechanism used in electrochemistry to describe the production of gas or the dissolution of metals:

$$\frac{\mathrm{d}}{\mathrm{d}t}\, x(t) = k_1(t)[1 - x(t)] - k_2(t)x(t), \qquad x(0) = \frac{k_1(0)}{k_1(0) + k_2(0)},$$

$$k_1(t) = p_1 \exp[p_2 u(t)], \qquad k_2(t) = p_3 \exp[p_4 u(t)],$$

$$y_{\mathrm{m}}(t) = k_1(t)[1 - x(t)] + k_2(t)x(t).$$

Differentiate observation equation with respect to time, to get

$$\frac{\mathrm{d}y_\mathrm{m}}{\mathrm{d}t} = \frac{\mathrm{d}k_1}{\mathrm{d}t}(1 - x) + \frac{\mathrm{d}k_2}{\mathrm{d}t}\, x + (k_2 - k_1)\frac{\mathrm{d}x}{\mathrm{d}t}\,.$$

Replace $\mathrm{d}x/\mathrm{d}t$ by its value as given by the state equation and multiply the result by $(k_2 - k_1)$ so as to use the observation equation to eliminate x and get the input-output equation

$$(k_2 - k_1)\frac{\mathrm{d}y_\mathrm{m}}{\mathrm{d}t} + [\frac{\mathrm{d}k_1}{\mathrm{d}t} - \frac{\mathrm{d}k_2}{\mathrm{d}t} + k_2^2 - k_1^2]\, y_\mathrm{m} = \frac{\mathrm{d}k_1}{\mathrm{d}t}\, k_2 - k_1\frac{\mathrm{d}k_2}{\mathrm{d}t} + 2k_1k_2(k_2 - k_1),$$

with the initial condition

$$y_\mathrm{m}(0) = k_1(0)[1 - x(0)] + k_2(0)x(0) = 2\,\frac{k_1(0)k_2(0)}{k_1(0) + k_2(0)}\,.$$

Exchanging k_1 and k_2 (*i.e.* (p_1, p_2) and (p_3, p_4)) leaves $y(0)$ unchanged and multiplies both sides of the input-output equation by (-1). $M(\cdot)$ is therefore not s.g.i.

Finally, consider a model defined by a set of relations

$$r_k(\mathbf{y}_\mathrm{m}, \mathbf{u}, \mathbf{x}, \mathbf{p}) = 0, \;\; k = 1, \ldots , n_\mathrm{r},$$

where the r_k's are polynomial functions of $\mathbf{u}$, $\mathbf{y}_\mathrm{m}$ and $\mathbf{x}$ and their derivatives with respect to time and polynomial functions of $\mathbf{p}$.

Any uniquely identifiable parameter p_k is the solution of a linear equation

$$a_k p_k = b_k,$$

where a_k and b_k are polynomial functions of the inputs, outputs and their derivatives with respect to time.

Computing a_k and b_k can therefore be used to prove the global identifiability of p_k.

Numerical local approach

The computations required by algebraic approaches prove sometimes too complex.

The following method can then be used to check whether $M(\cdot)$ is (at least locally) identifiable.

- Randomly pick $\mathbf{p}_0$ in $\mathbb{P}$ and simulate $M(\mathbf{p}_0)$ with a high precision to get fictitious data $\mathbf{y}^{\mathrm{f}}$.
- Estimate $\mathbf{p}$ from $\mathbf{y}^{\mathrm{f}}$ by minimizing a quadratic cost in the output error with a second-order method such as Newton or Gauss-Newton initialized at $\mathbf{p}_0$.
- If $\hat{\mathbf{p}}^{k}$ remains stable at $\mathbf{p}_0$, then M is s.l.i.
- If the estimator is unstable, this may have many causes. Other nominal values $\mathbf{p}_0$ should be picked before reaching a conclusion.

Optimization algorithms that incorporate a regularization procedure (such as Levenberg-Marquardt) cannot be used for testing local identifiability.

More sophisticated local numerical approaches can be used to study the local dependencies between unidentifiable parameters.

Distinguishability

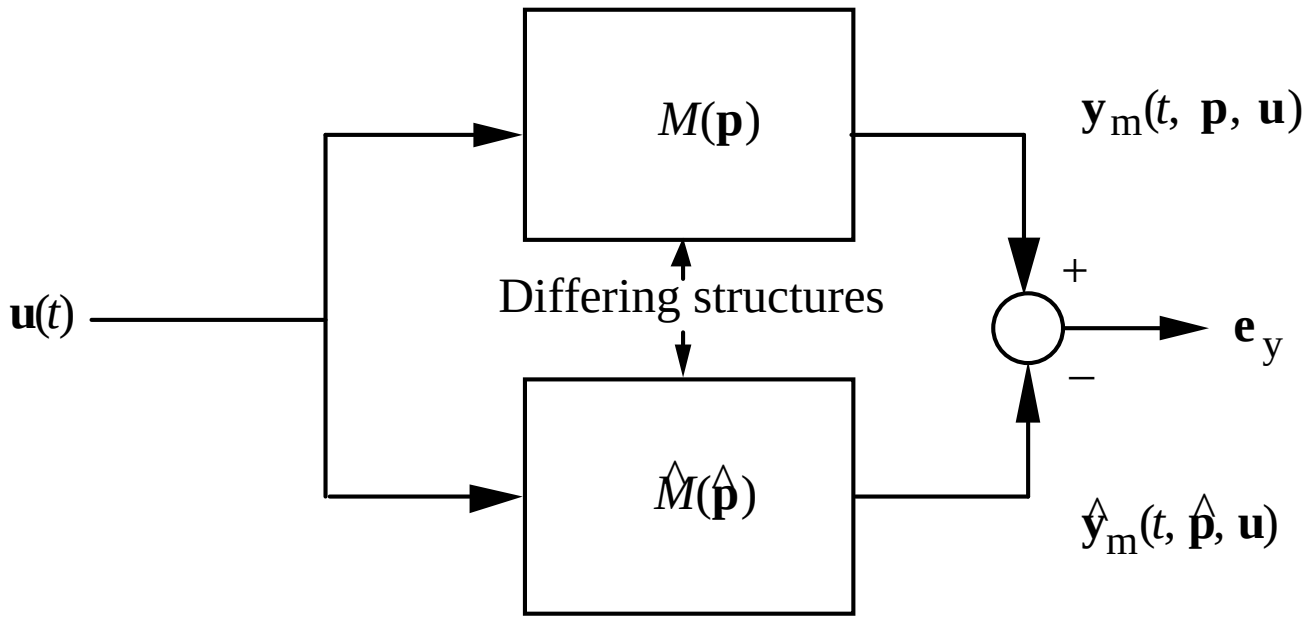
When hesitating between model structures, natural to ask whether the measurements will make it possible to decide which one is the best.

This question of distinguishability receives a partial answer in the same idealized framework as identifiability.

Assume the "process" is a model with structure $M(\cdot)$ while its "model" has the structure $\widehat{M}(\cdot)$, which now differs from $M(\cdot)$.

Let $\hat{\mathbf{p}}$ be the parameter vector associated with $\widehat{M}(\cdot)$, and $\mathbf{p}$ be the one associated with $M(\cdot)$.

It may be impossible to tune $\hat{\mathbf{p}}$ so that $\widehat{M}(\hat{\mathbf{p}}) = M(\mathbf{p})$. It is this impossibility that may permit the elimination of $\widehat{M}(\cdot)$ in favour of $M(\cdot)$.



$\hat{M}(\cdot)$ is *structurally distinguishable (s.d.) from* $M(\cdot)$ if, for almost any feasible value of $\mathbf{p}$, there is no feasible value of $\hat{\mathbf{p}}$ such that $\hat{M}(\hat{\mathbf{p}}) = M(\mathbf{p})$.

If $\hat{M}(\cdot)$ is s.d. from $M(\cdot)$ and *vice versa*, then $M(\cdot)$ and $\hat{M}(\cdot)$ are said to be s.d.

The techniques to test pairs of model structures for distinguishability are similar to those used for identifiability.

One now hopes to prove the non-existence of a solution for $\hat{\mathbf{p}}$, whereas in identifiability studies one hoped to prove the uniqueness of this solution.

EXAMPLE

$M(\cdot)$ defined by

$$\frac{\mathrm{d}}{\mathrm{d}t}\, x_1 = -(p_1+p_2)x_1 + p_3x_2 + u, \quad x_1(0) = 0,$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\, x_2 = p_2x_1 - p_3x_2, \quad x_2(0) = 0,$$
$$y_\mathrm{m} = x_1,$$

competes with $\widehat{M}(\cdot)$ defined by

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{x}_1 = -\hat{p}_2\hat{x}_1 + \hat{p}_3\hat{x}_2 + u, \quad \hat{x}_1(0) = 0,$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{x}_2 = \hat{p}_2\hat{x}_1 - (\hat{p}_1 + \hat{p}_3)\hat{x}_2, \quad \hat{x}_2(0) = 0,$$
$$\hat{y}_\mathrm{m} = \hat{x}_1.$$

Associated transfer functions, in the same canonical form:

$$H(s, \mathbf{p}) = \frac{s + p_3}{s^2 + s(p_1 + p_2 + p_3) + p_1p_3} \qquad \text{and} \qquad \hat{H}(s, \hat{\mathbf{p}}) = \frac{s + \hat{p}_1 + \hat{p}_3}{s^2 + s(\hat{p}_1 + \hat{p}_2 + \hat{p}_3) + \hat{p}_1\hat{p}_2}.$$

$\hat{M}(\hat{\mathbf{p}}) = M(\mathbf{p})$ thus translates into

$$\hat{p}_1 + \hat{p}_3 = p_3,$$
$$\hat{p}_1 + \hat{p}_2 + \hat{p}_3 = p_1 + p_2 + p_3,$$
$$\hat{p}_1\hat{p}_2 = p_1p_3.$$

For any $\mathbf{p}$, possible to find $\hat{\mathbf{p}}$ such that these equations are satisfied, and *vice versa*.

$M(\cdot)$ and $\widehat{M}(\cdot)$ are therefore structurally indistinguishable.

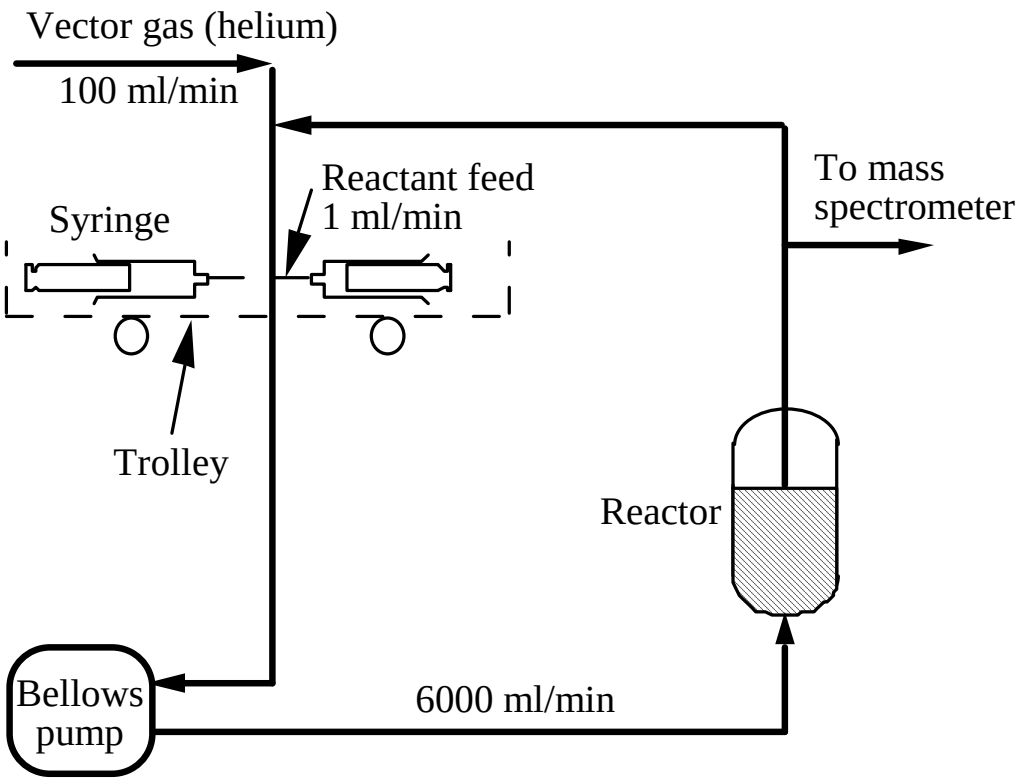
Impossible to know whether the structure chosen was right.

A possible way of removing ambiguity would be to monitor x_2.

REMARKS

- As for identifiability, there are cases where no structural conclusion can be drawn.
- Easy to prove that identifiability of two structures is neither necessary nor sufficient for their distinguishability.

Chemical engineering example



used to study reaction $CO + 3\,H_2 \rightleftharpoons CH_4 + H_2O$.

Prior considerations suggest two competing model structures:

$M(\cdot)$ defined by

$$C_1 \frac{\mathrm{d}}{\mathrm{d}t} x_1 = -(V + v_\mathrm{e})x_1 + v_\mathrm{e}x_2 + Vu,$$
$$C_2 \frac{\mathrm{d}}{\mathrm{d}t} x_2 = v_\mathrm{e}x_1 - v_\mathrm{e}x_2,$$
$$C_3 \frac{\mathrm{d}}{\mathrm{d}t} x_3 = Vx_1 - Vx_3,$$
$$C_4 \frac{\mathrm{d}}{\mathrm{d}t} x_4 = Vx_3 - Vx_4,$$
$$y_\mathrm{m} = x_4,$$

where the parameters to be estimated are $\mathbf{p} = (C_1, C_2, C_3, v_\mathrm{e})^\mathrm{T}$, and where V and C_4 are known from independent measurements.

$\widehat{M}(\cdot)$ defined by

$$C_1 \frac{\mathrm{d}}{\mathrm{d}t} \hat{x}_1 = -V\hat{x}_1 + Vu,$$

$$C_2 \frac{\mathrm{d}}{\mathrm{d}t} \hat{x}_2 = v_1\hat{x}_1 - v_1\hat{x}_2,$$

$$C_3 \frac{\mathrm{d}}{\mathrm{d}t} \hat{x}_3 = (V - v_1)\hat{x}_1 + v_1\hat{x}_2 - V\hat{x}_3,$$

$$C_4 \frac{\mathrm{d}}{\mathrm{d}t} \hat{x}_4 = V\hat{x}_3 - V\hat{x}_4,$$

$$\hat{y}_{\mathrm{m}} = \hat{x}_4,$$

where the parameters to be estimated are $\hat{\mathbf{p}} = (C_1, C_2, C_3, v_1)^{\mathrm{T}}$.

The state variables x_i and $\hat{x}_i$ ($i = 1, \ldots, 4$) are specific activities (percentages of labelled atoms), the C_i ($i = 1, \ldots, 3$) are surface concentrations and v_{e} and v_1 are flow rates of carbon atoms between adsorbed species.

All parameters and state variables therefore have a concrete meaning.

With the help of the Laplace-transform approach, the following conclusions can be reached:

- M and $\hat{M}$ are structurally indistinguishable,
- M is s.l.i. but not s.g.i. (three parameter vectors correspond to the same i/o behaviour),
- $\hat{M}$ is s.l.i. but not s.g.i. (six parameter vectors correspond to the same i/o behaviour).

One thus knows before any measurement that it will not be possible to find a best structure and unique best model within this structure.

Such model structures may nevertheless be of interest, provided that their ambiguous nature is recognized and taken into account.

Conclusions

Choosing a suitable model structure is not an exact science.

Testing structural properties, one can detect possible defects of the model structures considered even before data are available.

Identifiability is important when the parameters or state variables to be estimated have a concrete meaning or when decisions are to be taken on the basis of their numerical values.

The questions considered so far receive *qualitative answers* (yes / no / I do not know).

This raises a *quantitative question*: if $M(\cdot)$ is identifiable, what experiment should one perform to estimate its parameters as precisely as possible?

A first step will be to quantify identifiability. This is the subject of Unit 2.