Dynamic system modeling for control and diagnosis

Model verification, calibration and validation

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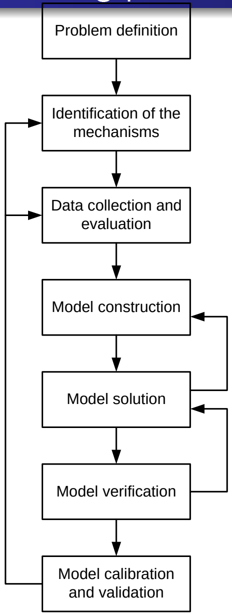
Lecture overview

1. Previous notions
2. Model solution and verification
3. The structure of state space models, structural analysis
   - Sign arithmetics
   - Model linearization
   - The structure of state space models
   - Structural properties
4. Statistical model calibration
   - Evaluation of the quality of the estimates
5. Statistical model validation

Recall: The 7 steps modeling procedure



Recall: The 7 steps modeling procedure

Steps to be discussed

6 Model verification
   - verifying qualitative model behavior against engineering intuition
   - checking dynamic properties (e.g. stability) on the model

7 Model calibration and validation
   - model calibration
     estimating unknown/uncertain model parameters
     using measured data
   - model validation
     comparing the model and the real system
     (measured data) using statistical methods

Solution of dynamic models

Assume: concentrated parameter model

- **Given**:
  - the model equations: systems of ordinary differential and algebraic equations (DAEs)
  - initial values
  - parameter values
- **Contstruct**: the solution of the model (time dependent values of the variables) system

Numerical solution methods: finite difference approximations, e.g. Runge-Kutta methods

Properties

- numerical stability (explicit vs. implicit methods)
- accuracy (the order of the method)
- automatic selection of the integration steps, stiff models

Model verification

Aim: verifying qualitative properties of the solution **against engineering intuition**

Model and/or solution properties

- steady states
  - existence, multiplicity
- *structural* dynamic properties
  - controllability and observability
  - (stability)
- qualitative properties of the step response
  - sign of initial deviation
  - steady state deviation

Model structure

The range set of signs

Universe: the range set of variables and constants

- *General qualitative*: real intervals with fixed or free end points

$$U_{\mathcal{I}} \;=\; \{[a_\ell, a_u] \mid a_\ell,\ a_u \in \mathcal{R},\ a_\ell \leq a_u\}$$

with the **landmark set**

$$L_{\mathcal{I}} = \{a_i \mid a_i \leq a_{i+1}\ ,\ i \in I \subseteq \mathcal{N}\}$$

- ***Sign***

$$\begin{aligned} U_{\mathcal{S}} &= \{\, + \,,\, - \,,\, 0 \,;\, ? \,\} \ ,\quad ? \;=\; + \cup 0 \cup - \\ L_{\mathcal{S}} &= \{\ a_1 = -\infty\ ,\ a_2 = 0\ ,\ a_3 = \infty\} \end{aligned}$$

- *Logical* (extended)

$$U_{\mathcal{L}} \;=\; \{\ \textbf{true}\ ,\ \textbf{false}\ ;\ \textbf{unknown}\ \}$$

Sign algebra

Algebra over the sign universe

Operations: with the **usual algebraic properties** (commutativity, associativity, distributivity)

- sign addition ($\oplus_S$) and substraction ($\ominus_S$)
- sign multiplication ($\otimes_S$) and division
- composite operations and functions

The specification (definition) of sign operations is done by using **operation tables**.

Sign addition

Operation table

$a \oplus_S b$	$+$	0	$-$	$?$
$+$	$+$	$+$	**?**	$?$
0	$+$	0	$-$	$?$
$-$	**?**	$-$	$-$	$?$
$?$	$?$	$?$	$?$	$?$

Properties:

- **growing uncertainty**
- commutative (symmetric over the main diagonal)

Sign multiplication

Operation table

$a \otimes_S b$	$+$	0	$-$	?
$+$	$+$	0	$-$	?
0	0	0	0	**0**
$-$	$-$	0	$+$	?
?	?	**0**	?	?

Properties:

- **correction** at zero operands
- commutative (symmetric over the main diagonal)

Models in nonlinear state space model form

Model originating from first engineering principles can be written in **state space model form**:

$$\begin{aligned} \frac{dx}{dt} &= F(x,u) \quad \text{(state eq.)} \\ y &= h(x,u) \quad \text{(output eq.)} \end{aligned}$$

where F and h are nonlinear functions.

Models from dynamic balance equations:

- state equations originate from the dynamic balance equations
- inputs and outputs depend also on measurement and actuating devices

Steady states

Steady state: x_0 is a given constant with identically constant (steady state) input u_0

For *input-affine systems*: we need to solve the equation below with a given to determine x_0

$$0 = f(x_0) + g(x_0)u_0 = F(x_0, u_0) \qquad (*)$$

$$y_0 = h(x_0)$$

$(*)$ may have more than one solution or no solution at all.

Centered variables: $\widetilde{x} = x - x_0$, $\widetilde{u} = u - u_0$

Linearization

Linearizing multivariate functions: $y = h(x_1, \ldots, x_n)$, $h : \mathcal{R}^n \mapsto \mathcal{R}^m$

$$\widetilde{y} = J^{(h,x)}\Big|_{x_0} \cdot \widetilde{x}$$

$$J_{ji}^{(h,x)} = \frac{\partial h_j}{\partial x_i}$$

where $J^{(h,x)}$ is the Jacobian matrix of h and $y_0 = h(x_0)$

Linearizing nonlinear state space models: one should linearize the nonlinear functions in the equations

$$\dot{x} = f(x) + g(x)u = F(x, u)$$

$$y = h(x)$$

around the steady state point (x_0, u_0).

Linearized state space models

Input-affine case: linearize the functions $\eta = F(x,u) = f(x) + g(x)u$ and $y = h(x)$ around the steady stat point (x_0, u_0)

$$\begin{aligned} \widetilde{y} &= \left. J^{(F,x)} \right|_{x_0,u_0} \cdot \widetilde{x} + \left. J^{(F,u)} \right|_{x_0,u_0} \cdot \widetilde{u} \\ \widetilde{y} &= \left(\left. J^{(f,x)} \right|_0 + \left. J^{(g,x)} \right|_0 u_0) \right) \cdot \widetilde{x} + g(x_0) \cdot \widetilde{u} \end{aligned}$$

LTI state space model form:

$$\begin{aligned} \dot{\widetilde{x}} &= \widetilde{A}\widetilde{x} + \widetilde{B}\widetilde{u} \\ \widetilde{y} &= \widetilde{C}\widetilde{x} + \widetilde{D}\widetilde{u} \end{aligned}$$

$$\widetilde{A} = \left. J^{(f,x)} \right|_0 + \left. J^{(g,x)} \right|_0 u_0, \quad \widetilde{B} = g(x_0), \quad \widetilde{C} = \left. J^{(h,x)} \right|_0, \quad \widetilde{D} = 0$$

The structure of state space models

Linearized state space models around a *steady state point*

$$\begin{aligned} \frac{dx}{dt} &= Ax + Bu \quad \text{(state eq.)} \\ y &= Cx + Du \quad \text{(output eq.)} \end{aligned}$$

for a nonlinear input-affine state space model

$$\begin{aligned} \frac{dx}{dt} &= f(x) + g(x)u \quad \text{(state eq.)} \\ y &= h(x) \quad \text{(output eq.)} \end{aligned}$$

Signed structure matrices: $[A]$

$$[A]_{ij} = \begin{cases} + & \text{if} \quad a_{ij} > 0 \\ 0 & \text{if} \quad a_{ij} = 0 \\ - & \text{if} \quad a_{ij} < 0 \end{cases}$$

Structure graph

Signed directed graph $S = (V, \mathcal{E}; w)$

- **vertex set** corresponds to state, input and output variables

$$V = X \cup U \cup Y$$
$$X \cap U = X \cap Y = U \cap Y = \emptyset$$

- **edges** correspond to *direct* effects between variables
- edge **weights** describe the *sign* of the effect

The occurrence matrix of a structure graph

An o_{ij} entry in the occurrence graph O

$$o_{ij} = \begin{cases} w_{ij} & ha \qquad\qquad (v_i, v_j) \in E \\ 0 & egyebkent \end{cases}$$

For a linear(ized) LTI state space model with (A, B, C, D) (order (u, x, y))

$$O = \begin{pmatrix} 0 & 0 & 0 \\ [B] & [A] & 0 \\ [D] & [C] & 0 \end{pmatrix}$$

For an input-affine SISO state space model

$$[A]_{ij} = \left[\frac{\partial f_i}{\partial x_j} + \frac{\partial g_i}{\partial x_j} u_0\right] \;,\; [B]_{i1} = [g_i]$$

$$[C]_{1j} = \left[\frac{\partial h}{\partial x_j}\right] \;,\; [D] = 0$$

Paths in the structure graph

A **directed path** $P = (v_1, v_2, ..., v_n)$, $v_i \in V$, $e_{i,i+1} = (v_i, v_{i+1}) \in \mathcal{E}$

- corresponds to the *indirect effect* of variable v_1 on variable v_n
- the *value* of the path is

$$W(P) = \prod_{i=1}^{n-1} w(e_{i,i+1})$$

- the significance of *shortest path(s)* and *directed circles*

Structural properties

Class of systems with the same structure: they have a state space model, the structure graph of which is the same

A system has a structural property if every element in the class of systems with the same structure - with a possible extension of a zero-measure set - has the property

Example: structural rank of matrices

$$s - rank \begin{pmatrix} 1 & 2 \\ 2 & 4 \end{pmatrix} = s - rank \begin{pmatrix} + & + \\ + & + \end{pmatrix} = 2$$

Structural controllability and observability

Structural properties: can be determined from the structure graph of a model
given by its signed structure matrices ($[A]$, $[B]$, $[C]$)

Structural controllability conditions

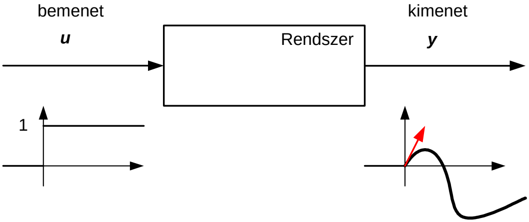
- $s - rank\ [A] = n$, i.e. $[A]$ is of full structural rank
- every state variable node is reachable from at least one input variable node in the structure graph via a directed path

Structural observability conditions

- $s - rank\ [A] = n$, i.e. $[A]$ is of full structural rank
- every state variable node is reachable from at least one output variable node in the structure graph via a directed path *with reversed direction*

Initial deviation of the unit step response – 1

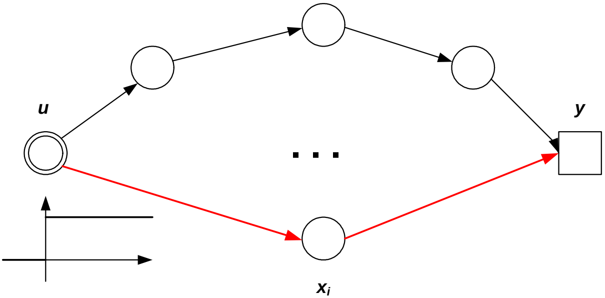
Unit step response



The sign value of the initial deviation is the sign value of the shortest path(s).

Initial deviation of the unit step response – 2

Sign-value of the shortest path(s!): more than one shortest path is possible



Deviation of the input (from its steady state value): $[\Delta u]_S = +$
Sign of the derivative: $[\frac{dx_i}{dt}]_S = \delta x_i = s_{u,x_i} \otimes_S [\Delta u]_S = s_{u,x_i}$
Sign of the **initial deviation** of the output:

$$[\frac{dy}{dt}]_S = \delta y = S^*_{u,y} \otimes_S [\Delta u]_S = s_{u,x_i} \otimes_S s_{x_i,y}$$

Model calibration – 1

Model Calibration – Conceptual Problem Statement

Given

- a grey-box model
- calibration data (measured data)
- measure of fit (loss function)

Compute

- an estimate of the parameter values and/or structural elements

Identification: dynamic model structure and parameter estimation

Model calibration – 2

Conceptual steps of solution

- Analysis of model specification
- Sampling of continuous time dynamic models
- Data analysis and preprocessing
- Model parameter and structure estimation
- Evaluation of the quality of the estimate

*The main tool of model calibration is **model parameter estimation**. We have learned about it in a separate **course "Parameter estimation"** in its part on **parameter estimation of dynamic models**.*

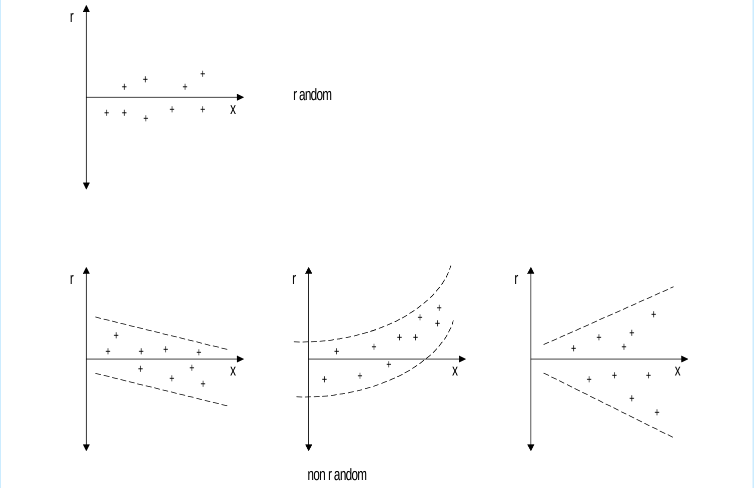
Recall: Steps of practical implementation of parameter estimation

Conceptual steps

- Preparing and checking measurement data
  - (Visual) overview of data: for serious error, outliers, trends
- Experiment design: choosing
  - proper sampling time
  - good number of samples
  - test signals for sufficient excitation
- Parameter estimation
- Evaluation of the quality of the estimates

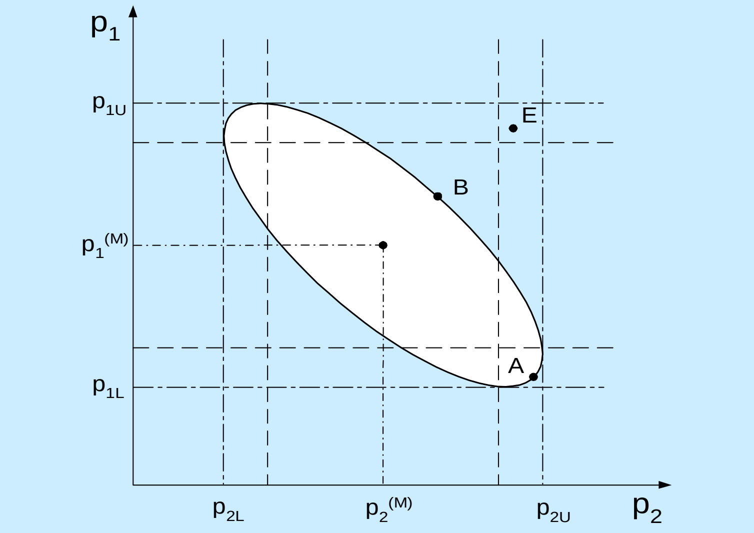
Evaluation of the quality of the estimates – 1

In the space of model outputs: ***residuals*** *should form white noise processes*



Evaluation of the quality of the estimates – 2

In the space of parameters: ***independent estimates*** *with low variance*



Statistical model validation

Conceptual problem statement

Given:

- a **calibrated** model
- validation data (measured data): independently measured from the calibration data (!!)
- measure of fit (loss function): in the space of output variables driven by the modelling goal

Decide (Question):

- Is the calibrated model "good enough" for the purpose (see modelling goal)?
  (Does it reproduce the data well?)