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Using Sequential Quadratic Programming for System Identification

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Abstract: System identification plays an important role in the development of process simulators and controllers. The ability to determine correctly the model parameters directly affects the model quality and, therefore, the model based controller performance. This work details the development of a system identification approach and its computational implementation based on sequential quadratic programming (SQP) in which first and second order linear systems, represented in state-space, are identified from simulated and from real industrial process data. Both single-input single-output and multivariable processes are considered. The resulting optimization problem may become not trivial to solve as one of the examples illustrates. It is shown how a rescaling of the decision variables or the use of a priori process knowledge may be used in order to overcome the difficulties and to improve the quality of the results.

Keywords: system identification, dynamical systems in control, multivariable systems, applications of mathematical programming

1 Introduction

A mathematical model is a representation of a real system that allows to predict its behavior in different scenarios. It should result in a compromise between realism and simplicity, i.e., it should incorporate most of the real system significant features yet it should not be so complex and difficult or even impossible to understand or experiment with [1]. Besides, an overly large number of parameters may be simply impossible to identify with the existing measurements.

System identification deals with the construction of mathematical models based on the experimental observation of the system response to some stimuli. Its use is widespread across all engineering fields (from aerospace, to civil or health industries [2,3,4]). It is also used for control purposes in the manufacturing and process industries. The operation of production lines has to be kept under control for economical and/or legal regulation reasons. The Proportional Integral Derivative (PID) controller is unquestionably the most common algorithm used in industry. In fact, more than 95% of the controllers used in industrial processes are the PID algorithm or its advanced versions [5,6,7]. In order to function properly, these controllers need to be tuned according to a specific performance criterion. A suboptimal tuning may result not only in undermined control performance but may also cause process instability [8,9].

The tuning of PID controllers requires a mathematical model of the process [10] of a sufficiently good quality. This notwithstanding, it is desirable to use the simplest possible model form as long as it is capable of capturing the most important steady-state and dynamic characteristics of the process [11].

Dynamic models derived from physical principles typically consist of one or more ordinary differential equations (ODE). Therefore, this kind of equations are also good candidate models for system identification purposes. The first order (FO), first order with time delay, and second order (SO) models are very useful to design and implement process controllers.

This article builds up on a previous work [12] for FO models, extends it to SO models, and exemplifies its applicability in both scenarios depending on the characteristics of the datasets.

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The FO model is defined as

$$\tau\,\dot{y}^*(t)+y^*(t)=K_p\,u^*(t)\,, \tag{1}$$

where y^* and u^* are the output observed variable and the input variable, respectively, both expressed via deviation variables, K_p is the static gain and τ is the time constant. The deviation variables y^* and u^* are related to the original variables y and u through a simple translation of the initial steady-state $\bar{y}$ and $\bar{u}$, respectively, that is,

$$y^*=y-\bar{y} \tag{2}$$

and

$$u^*=u-\bar{u}. \tag{3}$$

The static gain, K_p, represents how much the process output changes, from a steady-state to another, for a unitary variation of the process input while the time constant, τ, represents how fast the process responds to a change in the process input.

The SO model is mathematically described by

$$\ddot{y}^*(t)+2\xi\,\omega\,\dot{y}^*(t)+\omega^2\,y^*=K_p\,\omega^2 u^*(t)\,, \tag{4}$$

where ξ is the damping factor that determines the oscillatory behavior of the system, ω is the undamped natural frequency, and K_p is the gain of the system.

In simple processes, each output variable depends essentially on a single input variable. These may be modelled as the so called *single-input single-output* (SISO) systems. However, a large class of processes exhibits interaction among variables, i.e., each output variable is dependent on a subset of the input variables. These latter processes are regarded as *multiple-input multiple-output* (MIMO) systems. The common industrial practice is to assume that there is no interaction or to design controllers in a way that weakens the interaction. However, such approaches may result in suboptimal plant performance. Therefore, multivariable controller tuning, and thus, the multivariable system identification which is the subject of this work, have a big practical importance.

State-space models provide a compact and useful representation of a set of linear ODEs and can be generally written as

$$\begin{aligned}\dot{\mathbf{x}}(t)&=\mathbf{A}\,\mathbf{x}(t)+\mathbf{B}\,\mathbf{u}(t)\\ \mathbf{y}(t)&=\mathbf{C}\,\mathbf{x}(t)+\mathbf{E}\,\mathbf{u}(t)\end{aligned}\,, \tag{5}$$

where $\mathbf{x}(t)$ is the state vector, $\mathbf{u}(t)$ is the input variables vector, $\mathbf{y}(t)$ is the output vector of observed variables, and parameters $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$, and $\mathbf{E}$ are constant matrices of sizes $n_x\times n_x$, $n_x\times n_u$, $n_y\times n_x$ and $n_y\times n_u$, respectively. Typically, the observed variables are a subset of the state variables or a linear combination of them [13] and thus $\mathbf{E}$ is the null matrix.

System (5) may accommodate linear first order ODEs directly and higher order equations after a pre-treatment step in which higher order dynamics is represented by a set of first order equations [14,15]. In the particular case of a second order MIMO system, given in the form

$$\begin{aligned}\mathbf{M}\ddot{\mathbf{z}}(t)+\mathbf{D}\dot{\mathbf{z}}(t)+\mathbf{K}\mathbf{z}(t)&=\mathbf{F}\mathbf{u}(t)\\ \mathbf{y}(t)&=\mathbf{H}\mathbf{z}(t)\end{aligned}\,, \tag{6}$$

where $z\in\mathbb{R}^{n_z}$ and $\mathbf{M}$, $\mathbf{D}$, $\mathbf{K}$ ($\in\mathbb{R}^{n_z\times n_z}$), $\mathbf{F}$ ($\in\mathbb{R}^{n_z\times n_u}$), $\mathbf{H}$ ($\in\mathbb{R}^{n_y\times n_z}$) are constant matrices, it is possible to write equivalently that

$$\begin{aligned}\begin{bmatrix}\mathbf{I}&\mathbf{0}\\ \mathbf{0}&\mathbf{M}\end{bmatrix}\begin{bmatrix}\dot{\mathbf{z}}(t)\\ \ddot{\mathbf{z}}(t)\end{bmatrix}&=\begin{bmatrix}\mathbf{0}&\mathbf{I}\\ -\mathbf{K}&-\mathbf{D}\end{bmatrix}\begin{bmatrix}\mathbf{z}(t)\\ \dot{\mathbf{z}}(t)\end{bmatrix}+\begin{bmatrix}\mathbf{0}\\ \mathbf{F}\end{bmatrix}\mathbf{u}(t)\\ \mathbf{y}(t)&=\begin{bmatrix}\mathbf{H}&\mathbf{0}\end{bmatrix}\begin{bmatrix}\mathbf{z}(t)\\ \dot{\mathbf{z}}(t)\end{bmatrix}\end{aligned}\,, \tag{7}$$

where $\mathbf{I}$ and $\mathbf{0}$ represent the identity matrix and the zero matrix of appropriate sizes, respectively. Therefore,

$$\begin{aligned}\underbrace{\begin{bmatrix}\dot{\mathbf{z}}(t)\\ \ddot{\mathbf{z}}(t)\end{bmatrix}}_{\dot{\mathbf{x}}(t)}&=\underbrace{\begin{bmatrix}\mathbf{0}&\mathbf{I}\\ -\mathbf{M}^{-1}\mathbf{K}&-\mathbf{M}^{-1}\mathbf{D}\end{bmatrix}}_{\mathbf{A}}\underbrace{\begin{bmatrix}\mathbf{z}(t)\\ \dot{\mathbf{z}}(t)\end{bmatrix}}_{\mathbf{x}(t)}+\underbrace{\begin{bmatrix}\mathbf{0}\\ \mathbf{M}^{-1}\mathbf{F}\end{bmatrix}}_{\mathbf{B}}\mathbf{u}(t)\\ \mathbf{y}(t)&=\underbrace{\begin{bmatrix}\mathbf{H}&\mathbf{0}\end{bmatrix}}_{\mathbf{C}}\underbrace{\begin{bmatrix}\mathbf{z}(t)\\ \dot{\mathbf{z}}(t)\end{bmatrix}}_{\mathbf{x}(t)}\end{aligned}\,. \tag{8}$$

The first step of system identification consists of the so-called *process activation*. During this procedure the process is subjected to a set of disturbances whose magnitude should be carefully chosen. Indeed, if the process is activated too aggressively, the product quality may not be acceptable or the process safety may not be guaranteed. On the other hand, if the activation is not enough, an accurate process model cannot be obtained because the information included in the activated data is limited and the uncertainties (due for example to measurement noise and disturbances) may become dominant [16,17].

In the present work, a methodology for identification of systems in the process industry is presented. The procedure consists on minimizing the mismatch between the candidate model prediction and the actual response of the system, obtained after an adequate stimulation of the system. The process activation is performed through the use of a series of stepwise input signals in open loop scenarios. The optimization is performed via SQP technique. The developed tool can play an important role in designing and tuning the controllers needed in industrial environments.

2 Problem formulation

Once process data with sufficient information content is collected, the model parameters are determined such that

the model response reproduces the observed response of the actual process.

The most frequently used curve fitting criterion is the least squares criterion which minimizes the standard deviation of the model predictions from the dataset. Another common criterion is the sum of the absolute deviation. However, the latter is not continuous and that poses additional challenges in the optimization problem. The Chebyshev approximation criterion minimizes the largest absolute deviation over the entire set. However, this criterion is often difficult to apply in practice since the resulting optimization problem may require advanced mathematical procedures [18].

The nonlinear constrained optimization problem is defined as

$$\begin{aligned}
\underset{\mathbf{p}}{\text{minimize}} \quad & J(\mathbf{y},\mathbf{u},\mathbf{p}) && \text{(9a)}\\
\text{subject to} \quad & \dot{\mathbf{y}} = f(\mathbf{y},\mathbf{u},\mathbf{p}) && \text{(9b)}\\
& \mathbf{y}_{\mathrm{L}} \leq \mathbf{y} \leq \mathbf{y}_{\mathrm{U}} && \text{(9c)}\\
& \mathbf{u}_{\mathrm{L}} \leq \mathbf{u} \leq \mathbf{u}_{\mathrm{U}} && \text{(9d)}\\
& \mathbf{p}_{\mathrm{L}} \leq \mathbf{p} \leq \mathbf{p}_{\mathrm{U}} && \text{(9e)}\\
& g(\mathbf{p}) \leq 0, && \text{(9f)}
\end{aligned}$$

where J denotes the objective function, $\mathbf{p}$ is the model parameters vector to be estimated, $\mathbf{x}$ and $\mathbf{u}$ are the vectors of state and input variables (respectively), and the subscripts $_{\mathrm{L}}$ and $_{\mathrm{U}}$ stand for lower and upper (respectively). The set of equations (9b) defines a set of constraints arising from the model dynamics. Inequalities (9f) may enforce additional identification criteria.

Given a model $\mathbf{y} = f(\mathbf{y},\mathbf{u},\mathbf{p}) \in \mathbb{R}^{n_y}$ and a set of $m \times n_y$ data points $(t_i, \mathbf{y}_{\mathrm{exp},i})$, the objective function J is written, according to the minimum least squares criterion, as

$$J = \sum_{i=1}^{m} \left[\mathbf{y}_{\mathrm{exp},i} - \mathbf{y}_i\right]^{\top} \mathbf{Q} \left[\mathbf{y}_{\mathrm{exp},i} - \mathbf{y}_i\right], \qquad (10)$$

where $\mathbf{Q}$ is a diagonal matrix containing the weights given to each observed variable. In this work, equal weight was given to all output variables and thus $\mathbf{Q}$ is the $n_y \times n_y$ identity matrix.

It should be noted that generally (9) may become nonconvex causing numerical difficulties and local minima. However, since in this work the parameters belong to a linearized model and the number of the decision variables is low, the Sequential Quadratic Programming (SQP) exhibited satisfactory performance. Further solution refinement may be achieved via multistarting.

3 Results and discussion

3.1 SISO systems identification

An industrial heat exchanger installed in a process plant may be regarded as a SISO system. It was stimulated with a sequence of input steps and the profiles of the input and the output variables were registered. The obtained dataset contains 1200 points covering an interval of 100 minutes with a sampling period of 5 seconds. For confidentiality reasons the data was later normalized.

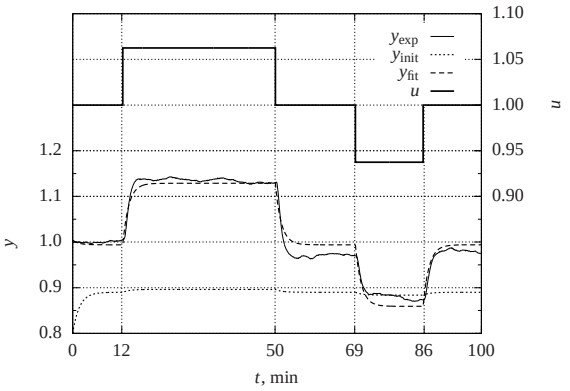

Fig. 1: SISO system identification using an FO model.

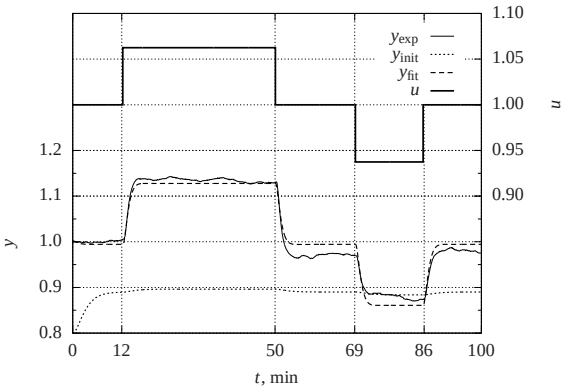

Fig. 2: SISO system identification using an SO model.

Both the stimuli, u, and the system response, y_{exp}, obtained during the process activation stage may be seen in Figure 1 (as well as in Figure 2). The success of system identification strongly depends on the quality of the data and, therefore, on its signal to noise ratio (SNR). The collected industrial dataset is characterized by an SNR of 11.0.

The optimization procedure described above was used to identify the system. The implementation was made in GNU Octave 3.6.3 using its general nonlinear minimization via `sqp()` successive quadratic programming solver. Based on the shape of the experimental response curve, both FO and SO models were tested (see (1) and (4)). The set of optimization related conditions and the obtained model parameters as well as some fitting quality indicators are presented in Table 1.

Table 1: Identification results for the SISO system using both FO and SO models.

p	Initial	LB	UB	Fit	Indicators
FO model					
K_p	0.100	0.0001	5	2.154	
τ	100.000	1	1000	88.868	$J = 0.286$
$\bar{x}$	0.800	−10	10	1.004	$R^2 = 0.9727$
$\bar{u}$	0.100	−10	10	1.005	
SO model					
K_p	0.100	0.0001	5	2.133	
ω	0.010	0	1	0.022	$J = 0.263$
ξ	1.000	0.0001	10	0.919	$R^2 = 0.9749$
$\bar{x}$	0.800	−10	10	1.002	
$\bar{u}$	0.100	−10	10	1.004	

Data set has SNR=11.0

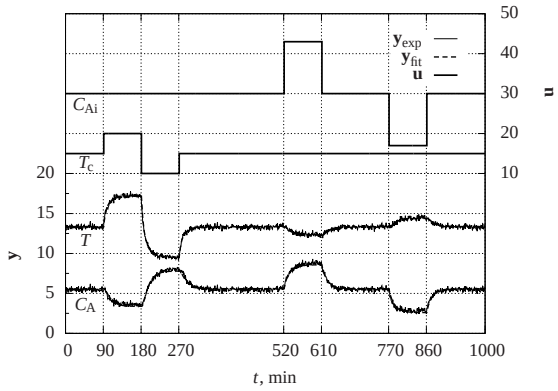

Fig. 3: MIMO system identification using an FO model.

The optimization tolerance was 10^{-6} in both cases (FO and SO). The dynamic responses of the mentioned models are drawn in Figures 1 and 2 (dashed line) for comparison with the real system response (thin solid line).

It is noteworthy that the SNR of the data is relatively significant and that the initial guess for the parameters is poor (as it is shown by the dotted line representing the model prediction with the first iteration parameters). Although these two factors make the identification process more difficult, both FO and SO resulting models are able to capture well the process dynamics, as proven by the high correlation factors, R^2.

Both models present a comparable performance, attested by similar values of the objective function and also by similar values of R^2 (see Table 1). By comparison of Figures 1 and 2, it is possible to conclude that the predictions of both models are, in this case, quite similar.

Therefore, and in this specific situation, we select the FO model since it is able to achieve the same performance as the SO model but with a simpler structure. The lower number of parameters of the FO model also reduces the computational effort required in the fitting.

3.2 MIMO systems identification

A continuous stirred tank reactor (CSTR) equipped with a heating coil is a good example of a MIMO system commonly used in industry. This system has two input variables (the inlet flow concentration of reactant A, $C_{A,i}$, and the temperature of the heating fluid in the coil, T_c) and two output variables (the concentration of reactant in the reactor, C_A, and the temperature in the reactor, T).

In order to collect data for the identification of a CSTR subjected to external heating, a plant simulation was carried out using the first principles ODE model (Appendix A). The timespan of the data is 1000 minutes with a sampling interval of 1 min. This data set exhibits SNR of 8.6 and 3.8 for T_{exp} and $C_{A,exp}$, respectively.

The input used to stimulate the system and the generated experimental results are plotted in Figure 3.

The interaction among the variables is clear: for instance, a disturbance in input variable T_c results in a dynamic response not only of T but also of the second output variable, C_A. Similarly, by activating the input variable $C_{A,i}$ both output variables are affected.

First order model:

Using an FO model whose state variables vector coincide with the output variables vector $\mathbf{x}(t) = \mathbf{y}(t) = \left[T\ C_A\right]^\top$, all **A**, **B**, and **C** matrices have dimension 2×2 and matrix **C** is the identity matrix. Also, from an a priori physical/chemical analysis of the system, it is possible to conclude that the first input variable (T_c) has a direct effect on T while it has an indirect effect on C_A through the variable T. Moreover, it is possible to perceive that the effect of the second input variable ($C_{A,i}$) is direct on C_A but indirect on T. These facts can be used to reduce to 10 the number of parameters to be estimated through optimization for the FO model, since $\mathbf{B}_{12} = \mathbf{B}_{21} = 0$.
The parameter values of this system determined by the optimization technique under a tolerance of 10^{-6} are summarized in Table 2.
In spite of the high level of noise, especially in the second variable (SNR $= \left[8.6\ 3.8\right]$), the obtained correlation factor was even higher than in the case of the SISO system, revealing an excellent fit quality. The model response with the optimized parameters is drawn (dashed line) in Figure 3 together with the experimental response of the system (thin solid line) for easy comparison. The model is able to capture the peculiarities of the system, namely the strong interactions among its variables.

Second order model:

Table 2: Identification results for the MIMO system using FO and SO models.

p	Initial	LB	UB	Fit	Indicators
FO model					
$\mathbf{A}_{11}$	$-1{\cdot}10^{-2}$	-1	1	$-0.280{\cdot}10^{-2}$	
$\mathbf{A}_{12}$	$-1{\cdot}10^{-3}$	-1	1	$-0.982{\cdot}10^{-3}$	
$\mathbf{A}_{21}$	$-1{\cdot}10^{-3}$	-1	1	$-1.074{\cdot}10^{-3}$	
$\mathbf{A}_{22}$	$-1{\cdot}10^{-2}$	-1	1	$-0.186{\cdot}10^{-2}$	
$\mathbf{B}_{11}$	$1{\cdot}10^{-3}$	-1	1	$1.709{\cdot}10^{-3}$	J = 99.215
$\mathbf{B}_{22}$	$1{\cdot}10^{-3}$	-1	1	$0.341{\cdot}10^{-3}$	R^2 = 0.9971
$\bar{\mathbf{x}}_1$	15	0	45	13.247	
$\bar{\mathbf{x}}_2$	1	0	45	5.353	
$\bar{\mathbf{u}}_1$	20	1	100	14.714	
$\bar{\mathbf{u}}_2$	25	1	100	28.416	
SO model					
$\mathbf{A}_{31}$	$-5{\cdot}10^{-5}$	-1	1	$-5.248{\cdot}10^{-5}$	
$\mathbf{A}_{32}$	$-2{\cdot}10^{-6}$	-1	1	$-18.47{\cdot}10^{-6}$	
$\mathbf{A}_{33}$	$-2{\cdot}10^{-2}$	-1	1	$-2.041{\cdot}10^{-2}$	
$\mathbf{A}_{34}$	$-2{\cdot}10^{-3}$	-1	1	$-2.034{\cdot}10^{-3}$	
$\mathbf{A}_{41}$	$-2{\cdot}10^{-6}$	-1	1	$-19.51{\cdot}10^{-6}$	
$\mathbf{A}_{42}$	$-1{\cdot}10^{-5}$	-1	1	$-3.369{\cdot}10^{-5}$	
$\mathbf{A}_{43}$	$-2{\cdot}10^{-3}$	-1	1	$-1.683{\cdot}10^{-3}$	J = 110.579
$\mathbf{A}_{44}$	$-2{\cdot}10^{-2}$	-1	1	$-1.958{\cdot}10^{-2}$	R^2 = 0.9968
$\mathbf{B}_{31}$	$-9{\cdot}10^{-6}$	-1	1	$31.60{\cdot}10^{-6}$	
$\mathbf{B}_{42}$	$-9{\cdot}10^{-6}$	-1	1	$6.125{\cdot}10^{-6}$	
$\bar{\mathbf{x}}_3$	15	0	45	13.314	
$\bar{\mathbf{x}}_4$	1	0	45	5.416	
$\bar{\mathbf{u}}_1$	20	1	100	14.857	
$\bar{\mathbf{u}}_2$	25	1	100	28.961	

Data set has SNR=$\begin{bmatrix}8.6 & 3.8\end{bmatrix}$

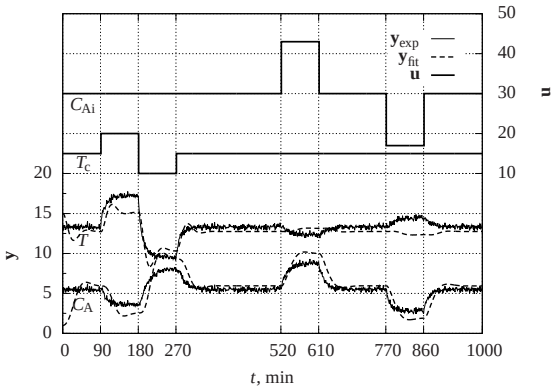

Fig. 4: Difficulties in identifying the MIMO system via an SO model.

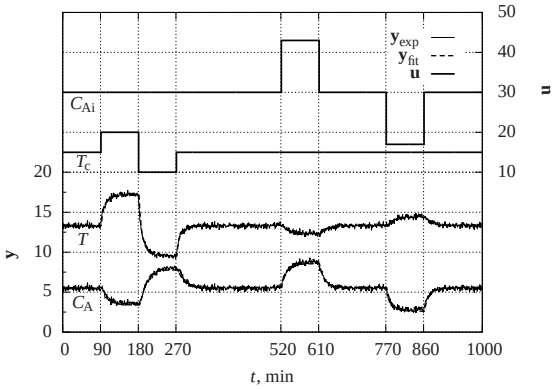

Fig. 5: MIMO system identification using an SO model.

In the present article, the identification of the MIMO system is also carried out via an SO approach. The state variables vector was defined as $\mathbf{x}(t) = \begin{bmatrix}T & C_\mathrm{A} & \dot{T} & \dot{C_\mathrm{A}}\end{bmatrix}^\top$ and thus the observed (measured) variables coincide with a subset of the state variables, T and C_A. In such situation: (i) the dimensions of matrices **A**, **B** and **C** (see (5)) are 4×4, 4×2 and 2×4, respectively; (ii) **C** is constituted exclusively by 0 and 1 elements: the **H** part of **C** (see (8)) is the 2×2 identity matrix; (iii) the two first rows of **A** as well as the two first rows of B are 0 except the elements $\mathbf{A}_{13}$ and $\mathbf{A}_{24}$ which are 1. For the reasons also invoked when applying the FO model to this system, elements $\mathbf{B}_{31}$ and $\mathbf{B}_{42}$ were set to 0. The initial steady-state value for the state variables $\dot{T}$ and $\dot{C_\mathrm{A}}$ was equally set to zero since both T and C_A are constant at steady-state. Therefore, the number of parameters needed to be estimated for the SO model applied to the MIMO system is 14.

According to (9), simultaneous accounting of both output curves of the MIMO system was considered during the optimization process (ie, the objective function was the sum of 2×1000 square errors between original and predicted values), both when using the FO model (see above) or the SO model.

In the first attempt, the optimization algorithm encountered more difficulties in finding the parameters of this model. Even when the tolerance was decreased to 10^{-10}, the resulting model presented bad prediction performance (Figure 4) with $R^2 = 0.9323$ and $J = 2430.979$, which is frankly worse than that achieved with the FO model ($R^2 = 0.9971$ and $J = 99.215$).

This unacceptable fit quality was caused by poor conditioning of the data. Since the tolerance values were already relatively close to the machine precision, the parameters were equally scaled up by a 10^8 factor, with the necessary changes in the model. This approach proved effective as the resulting fit is as good as that obtained for the FO model. These parameters are listed in Table 2 and the corresponding model response can be observed in Figura 5.

The SO model is now able to reproduce the system response in a comparable way to the FO model (compare Figures 5 and 3 and values of J and R^2 in Table 2).

Since the performance of FO and SO models are comparable, the FO model is preferable as it represents the best trade-off between performance and simplicity.

4 Conclusions

A system identification tool for SISO and MIMO models was developed using the Sequential Quadratic Programming algorithm. The performance of the approach was tested using datasets from both a real industrial process (SISO system) and from a simulated process unit (MIMO system). The resulting models reproduce well the experimental data and, thus, may be used for process simulation and/or control system design.

For the SISO systems, it was possible to obtain FO and SO models of comparable performance. Therefore, the FO model was adopted for both systems as it has a simpler structure and requires less parameters.

For the MIMO system, the FO model parametrized via optimization reproduced quite well the experimental data. The optimizer showed some difficulties to parametrize an SO model for this system. However, such solution existed and was found by scaling up the parameters to be optimized in order to increase the sensitivity of the optimizer to them. The optimization solution corresponding to the MIMO system revealed to be sensitive to the initial estimate. Thus, the FO model was considered to be the most adequate for the MIMO system.

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A Appendix A – CSTR model

Consider a simple liquid phase reactor where an irreversible first order chemical reaction takes place converting reactant A to product B. The inlet stream consists of pure component A with molar concentration C_{Ai}. A heating coil is used to maintain the reaction mixture at the desired operating temperature by adding heat needed for the endothermic reaction to take place.

A deterministic mathematical model can be built based on the following assumptions:

Table 3: CSTR model parameters.

Parameter	Value	Unit
A_t	9.7980	m^2
c_p	1033.78	$J\,kg^{-1}\,{}^\circ C^{-1}$
E_a/R	$1.0838{\cdot}10^4$	$^\circ C$
k_0	$4.0{\cdot}10^{13}$	s^{-1}
q	0.0013	$m^3\,s^{-1}$
T_i	50	$^\circ C$
U	500	$W\,m^{-2}\,{}^\circ C^{-1}$
V	3.7854	m^3
ΔH	$5.0{\cdot}10^5$	$J\,mol^{-1}$
ρ	832.96	$kg\,m^{-3}$

– the CSTR is perfectly mixed;
– the reaction rate can be defined through Arrhenius equation: $k = k_0 \exp(-\frac{E_a}{R\,T})$, where k_0 is the frequency factor, E_a is the activation energy and R is the gas constant;
– the mass densities, ρ, and the specific heat capacity, c_p, of the feed and product streams are equal and constant;
– the liquid volume, V, in the reactor is kept constant;
– the thermal capacitances of the heating fluid and of the coil wall are negligible compared to the thermal capacitance of the liquid in the tank;
– all the heating fluid is at a uniform temperature, T_c;
– the rate of heat transfer from the heating fluid to the reacting mixture is given by $UA_t(T_c - T)$ where U is the overall heat transfer coefficient and A_t is the heat transfer area.

Material and energy balance equations may be rearranged into

$$V\,\frac{dC_A}{dt} = q(C_{Ai} - C_A) - VkC_A\ , \tag{11a}$$

$$V\rho c_p\,\frac{dT}{dt} = q\rho c_p(T_i - T) + (-\Delta H)VkC_A + UA_t(T_c - T)\ . \tag{11b}$$

The model parameters were adapted from exercise 4.14 of [13] and are listed in Table 3.

The set of differential equations defined by (11) was implemented in GNU Octave [19] and integrated using LSODE solver [20] for a series of different steps in the input variables profiles and with a finite-differences approximation of the derivative information. More details about it can be found in [21]. The outputs of the model, corrupted with a random noise, constitute the experimental data set for the identification of the MIMO system.

Nomenclature

$\mathbf{A}$	state-space model constant matrix	s^{-1}
A_t	heat transfer area	m^2
$\mathbf{B}$	state-space model constant matrix	$[\mathbf{x}]\,[\mathbf{u}]^{-1}\,s^{-1}$
c_p	specific heat capacity at pressure constant of the liquid	$J\,kg^{-1}\circ C^{-1}$
$\mathbf{C}$	state-space model constant matrix	$[\mathbf{y}]\,[\mathbf{x}]^{-1}$
C_A	concentration of the reactant A in the reactor	$mol\,m^{-3}$
C_{Ai}	inlet flow concentration of the reactant A	$mol\,m^{-3}$
E_a	activation energy	$J\,mol^{-1}$
J	objective function	dimensionless
k_0	frequency factor	s^{-1}
k	pre-exponential factor of Arrhenius's Law	s^{-1}
K_p	static gain	$[x]\,[u]^{-1}$
m	number of sampling times	dimensionless
n_x	number of state variables	dimensionless
n_y	number of observed variables	dimensionless
n_u	number of input variables	dimensionless
$\mathbf{p}$	model parameters vector	$[\mathbf{p}]$
q	flow through the tank	$m^3\,s^{-1}$
$\mathbf{Q}$	matrix of weights in the optimization	$[y]^{-2}$
R	ideal gas constant	$J\,mol^{-1}\circ C^{-1}$
T	temperature in the reactor	$\circ C$
T_i	temperature of the inlet liquid flow	$\circ C$
T_c	temperature of the heating fluid in the coil	$\circ C$
u	input variable	$[u]$
u^*	deviation input variable	$[u]$
$\bar{u}$	initial steady-state input variable	$[u]$
$\mathbf{u}$	input variables vector	$[\mathbf{u}]$
$\mathbf{u}^*$	deviation input variables vector	$[\mathbf{u}]$
$\bar{\mathbf{u}}$	initial steady-state input variables vector	$[\mathbf{u}]$
U	overall heat transfer coefficient	$W\,m^{-2}\circ C^{-1}$
V	volume of the liquid in the tank	m^3
x	state variable	$[x]$
x^*	deviation state variable	$[x]$
$\bar{x}$	initial steady-state state variable	$[x]$
$\mathbf{x}$	state variables vector	$[\mathbf{x}]$
$\mathbf{x}^*$	deviation state variables vector	$[\mathbf{x}]$
$\bar{\mathbf{x}}$	initial steady-state state variables vector	$[\mathbf{x}]$
y	observed (also called output or measured) variable	$[y]$
y^*	deviation observed variable	$[y]$
$\bar{y}$	initial steady-state observed variable	$[y]$
$\mathbf{y}$	observed variables vector	$[\mathbf{y}]$
$\mathbf{y}^*$	deviation observed variables vector	$[\mathbf{y}]$
$\bar{\mathbf{y}}$	initial steady-state observed variables vector	$[\mathbf{y}]$
ΔH	heat of reaction	$J\,mol^{-1}$
ξ	damping factor	dimensionless
ρ	mass density of the liquid	$kg\,m^{-3}$
τ	time constant	s
ω	undamped natural frequency	s^{-1}

Subscripts

A	relative to reactant A
exp	experimental
fit	fitting
L	lower bound
U	upper bound

Acronyms

FO	First Order model
LB	Lower Bound
MIMO	Multiple-Input Multiple-Output system
ODE	Ordinary Differential Equation
PID	Proportional-Integral-Derivative controller
SISO	Single-Input Single-Output system
SNR	Signal to Noise Ratio
NR	Signal to Noise Ratio
SO	Second Order model
SQP	Sequential Quadratic Programming
UB	Upper Bound

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