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Identification of Ill-Conditioned Systems Using Output Rotation

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Abstract: A new method for identification of ill-conditioned systems is suggested. Our aim is to provide a solution that is practical and functional in the sense that no initial knowledge about process is needed, light-weight tools can be used for identification (e.g. simple ARX models with standard least-squares regression), and model structures with minimal number of parameters and states are used. The main idea is to employ principal component analysis (PCA) to rotate the outputs before identifying the process in directions important for control.

Keywords: Identification for control, Process modeling and identification, Ill-conditioned systems, Principal Component Analysis, Process directionality, Distillation control

1. INTRODUCTION

Many industrial multi-variable controllers (e.g. Model-Predictive Control, MPC) are model-based, i.e. some kind of model of the controlled process is utilized by the controller. The usage of model-based controllers have increased during the last decades because there is a continuous need for faster, more accurate, and more robust controllers, as new standards are continuously set for flexibility of operation and economic efficiency. An important, but costly step in model-based control is process identification which must be done regularly to keep the model up to date and control performance at an acceptable level.

A multi-variable process may be ill-conditioned, which is seen as a high condition number of the steady-state gain matrix. Ill-conditioned processes are not rare in the process industry. For example, high-purity distillation columns are practically always ill-conditioned. Ill-conditioned processes are characterized by directionality, i.e. some input directions are highly amplified, and some are not. In addition, process dynamics usually go hand in hand with the gain directions. For distillation models (Skogestad and Morari (1988)) it is known that the high gain direction is considerable slower than the low gain direction. According to Häggblom (2014), this observation holds generally, and high gain directions are slower than low gain directions. Standard identification experiments that neglect directionality generate trends with fast dynamics hidden in the responses. As a result, the model fit looks good, and poor models are not revealed before they are validated in the low-gain direction.

There are some practical problems associated with identification of ill-conditioned systems. According to Jacobsen and Skogestad (1994), we should identify some two-pole-one-zero transfer function elements to capture both the fast and slow dynamics of a 2×2 system. From a practical point of view the high number of parameters are difficult to identify when there are noise and disturbances present during identification.

Improved identification of ill-conditioned systems can also be achieved by properly designing input excitation of the identification experiment (Häggblom, 2019a), (Häggblom, 2019b). This improves the identification results in all gain directions, which is crucial when the model is utilized for control and controller design.

An identification method applied on industrial processes must be practical and simple. The method used for identification should be able to evaluate the results of an identification experiment in an easy and understandable way, and preferably guide user in decision making. A simple parameter estimation method is preferred, as it may be implemented in the automation system instead of collecting data from the process and running the identification procedure on an office PC. Further, the method should be resistant to noise and disturbances that are always present during identification. For ill-conditioned processes it is important to ensure that we identify all gain directions, and capture the dynamics in all gain direction and that we can measure the quality of the identification in the low-gain direction.

It has been estimated that distillation stands for 10-15% of total energy consumption in the world, so tight distillation control can bring huge energy savings. Many distillation columns are controlled with advanced model-based controllers, like MPC. However, MPC can deliver improved control performance only when the models are up to date. Therefore, there is a need for an easy-to-implement, practical solution, which makes it easy to keep the MPC models up to date. We believe that the method presented in this paper will improve, speed up, and simplify identification of ill-conditioned processes and enable tight control of high-purity distillation.

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2. SUGGESTED METHOD

In this section we introduce a new method for identification of ill-conditioned processes, based on output rotation. We discuss some model structures suitable for the method. For simplicity, we assume that process is of size 2×2 but all concepts discussed here may be extended to larger systems as well.

We focus on practical solutions, so only simple models are used. With simple models, we mean that minimal number of states and parameters are used. Also, we assume that only linear least-squares parameter estimation of ARX models is used and that multi-variable models are identified one output at time. These restrictions ensure that the method is easy to implement in practice.

2.1 Modeling Directionality

Traditionally, high-purity distillation models have been obtained by fitting individual transfer function elements, typically first-ordered-plus-dead-time transfer functions for each input-output pair (Wood and Berry, 1973)(Waller et al., 1988)

$$\mathbf{G(s)} = \begin{pmatrix} \dfrac{k_{11}exp(-L_{11}s)}{T_{11}s+1} & \dfrac{k_{12}exp(-L_{12}s)}{T_{12}s+1} \\ \dfrac{k_{21}exp(-L_{21}s)}{T_{21}s+1} & \dfrac{k_{22}exp(-L_{22}s)}{T_{22}s+1} \end{pmatrix} \tag{1}$$

Jacobsen and Skogestad (1994) argue that such models are seemingly well fitted by open-loop data, but they exhibit inconsistent behavior when used for feedback control. The main problem is that the dynamics of the faster low gain dynamics is missing from the model. To capture the dynamics of a 2×2 system governed by directionality, Jacobsen and Skogestad (1994) suggest the model structure

$$\mathbf{G_{106}(s)} = \frac{\begin{pmatrix} k_{11}(z_{11}s+1) & k_{12}(z_{12}s+1) \\ k_{21}(z_{21}s+1) & k_{22}(z_{22}s+1) \end{pmatrix}}{(T_1 s+1)(T_2 s+1)} \tag{2}$$

This model can capture both the slow responses in the high gain direction and the fast responses in the low gain direction. The model (2) is labeled G_{106} as it has 10 parameters and 6 states in the general case. The high number of parameters makes it difficult to identify when there are noise and disturbances present during identification.

Häggblom and Böling (1998) used a model similar to Eq. 1 but they increased the model order from first to second order dynamics, which must be done to capture the directionality of distillation columns. They used process knowledge to reduce the number of free parameters in the model by adding several constraints and relations between parameters. Such a model can not, however, be identified using simple linear regression.

To our knowledge, process identification has traditionally been made by identifying the model from physical inputs to physical outputs in one step. In this paper we use output rotation, and identify the process in parts. In the first step we identify a matrix, which rotates the outputs, and in the second step we identify a simplified model from physical inputs to rotated outputs. Finally, we combine the identified models and the rotation matrix to derive an input-output model.

The motivation behind using output rotation is that it simplifies the identification. We can reduce the number of parameters that we must estimate. Moreover, the rotated outputs are uncorrelated so we can identify the rotated outputs one at a time. These improvements simplifies and increases the reliability of the identification.

Output rotation is discussed below. Before that, we justify the use of rotated outputs and suggest some simple model structures for 2×2 ill-conditioned systems.

2.2 Simple Models of Ill-Conditioned Processes

As discussed above, Jacobsen and Skogestad (1994) suggested the model structure (2) for ill-conditioned systems where the ambition is to identify a model that can capture the dynamics in all gain directions. They state that "only two of the zeros may be adjusted independently as we require a model with only two states". With this two-state limitation we get a special case of model (2), which can be written as

$$\mathbf{G_{62}(s)} = \mathbf{W} \begin{pmatrix} \dfrac{k_1}{T_1 s+1} & 0 \\ 0 & \dfrac{k_2}{T_2 s+1} \end{pmatrix} \mathbf{V^T} \tag{3}$$

Here the matrices $\mathbf{W}$ and $\mathbf{V}$ can, for example, be obtained using SVD decomposition of the steady-state gain matrix

$$\mathbf{K} = \begin{pmatrix} k_{11} & k_{12} \\ k_{21} & k_{22} \end{pmatrix} = \mathbf{W} \begin{pmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{pmatrix} \mathbf{V^T} \tag{4}$$

Note the matrices $\mathbf{W}$ and $\mathbf{V}$, in Eq. (3) are not always strict rotation matrices as in Eq. (4), but they can also be obtained by scaling pure rotation matrices with a diagonal scaling matrix.

In this paper we consider some special cases of model (2) and draw attention to number of states and parameters. The simplest (unscaled) rotation matrix is specified with one parameter (the rotation angle), so the model G_{62} (Eq. 3) has two rotation angles, two time constants (T_1 and T_2), two gains (k_1 and k_2) and we need two states for simulation.

Usually, ill-conditioned processes are characterized by different dynamics in different gain directions. In cases where $T_2 << T_1$ we may further reduce the number of parameters and states by neglecting the dynamics of the low gain direction. With $T_2 = 0$, model (3) reduces to

$$\mathbf{G_{51}(s)} = \mathbf{W} \begin{pmatrix} \dfrac{k_1}{T_1 s+1} & 0 \\ 0 & k_2 \end{pmatrix} \mathbf{V^T} \tag{5}$$

Model G_{51} (Eq. 5) is very appealing from a practical point of view as it has only 5 parameters and one state.

2.3 Output Rotation

Next, we justify the use of output rotation. Assume that our task is to identify G_{62} (model 3) and that $\mathbf{W}$ is known. Then the rotated outputs can be identified one at a time as two-input-single-output first-order systems. If both $\mathbf{W}$ and $\mathbf{V}$ are known, then G_{62} can be identified from rotated inputs to rotated outputs, by identifying two single-input-single-output first-order systems.

The output rotation matrix $\mathbf{W}$ can be estimated in various ways. If an estimate of the steady-state gain matrix $\mathbf{K}$ is known, we can use SVD (Eq. 4) to calculate $\mathbf{W}$ and $\mathbf{V}$. On the other hand, if $\mathbf{K}$ is unknown, we can estimate $\mathbf{W}$ from output data using principal component analysis. This is discussed next.

Consider a zero mean input matrix $\mathbf{U}$ of size $n \times m$, organized such that each row is a sampling instant, and each column is an input signal. Further consider an output matrix $\mathbf{Y}$ of same size generated by a gain matrix $\mathbf{K}$ of size $m \times m$, i.e.

$$\mathbf{Y} = \mathbf{U}\mathbf{K}^{\mathbf{T}} \tag{6}$$

Next we introduce the dimensionless gain matrix $\mathbf{K}_0$ and

$$\mathbf{Y_0} = \mathbf{U_0}\mathbf{K_0^T} \tag{7}$$

where the dimensionless matrices $\mathbf{U}_0$ and $\mathbf{Y}_0$ have been obtained by scaling $\mathbf{Y}$ and $\mathbf{U}$ using the diagonal scaling matrices $\mathbf{K}_u$ and $\mathbf{K}_y$ as

$$\mathbf{U_0} = \mathbf{U}\mathbf{K_u} \tag{8}$$
$$\mathbf{Y_0} = \mathbf{Y}\mathbf{K_y^{-1}} \tag{9}$$

$\mathbf{K}_u$ and $\mathbf{K}_y$ are diagonal matrices with scaling constants on their diagonals. The purpose of scaling is to create a dimensionless gain matrix $\mathbf{K}_0$, which simplifies the analysis and better describes process directionality than the scale-dependent $\mathbf{K}$.

The dimensionless steady-state gain $\mathbf{K}_0$ is decomposed using singular value decomposition

$$\mathbf{K_0} = \mathbf{W_0}\mathbf{\Sigma_0}\mathbf{V_0^T} \tag{10}$$

Now we use PCA to rotate the outputs before identification. PCA is scaling-dependent, so we consider the principal components of the scaled output matrix $\mathbf{Y}_0$

$$\mathbf{T} = \mathbf{Y_0}\mathbf{P} \tag{11}$$

where $\mathbf{P}$ is an $m \times m$ matrix whose columns are the eigenvectors of the covariance matrix of $\mathbf{Y}_0$. Assume that the signals of $\mathbf{U}_0$ are uncorrelated with unity covariance (i.e. the inputs $\mathbf{U}$ are uncorrelated and the scaling matrix $\mathbf{K}_u$ is suitable selected). Then the covariance of $\mathbf{Y}_0$ is

$$cov(\mathbf{Y_0}) = \mathbf{K_0}cov(\mathbf{U_0})\mathbf{K_0^T} = \mathbf{K_0}\mathbf{K_0^T} \tag{12}$$

Now as stated above, the principal components are calculated from the eigenvectors of $cov(\mathbf{Y_0})$. The eigenvectors of $\mathbf{K_0}\mathbf{K_0^T}$ are the columns of $\mathbf{W_0}$ (Wikipedia contributors, 2019), and we get

$$\mathbf{P} = \mathbf{W_0} \tag{13}$$

The principal components of $\mathbf{Y}_0$ are

$$\mathbf{T} = \mathbf{Y_0}\mathbf{W_0} \tag{14}$$

Above we assumed steady-state relations but if we assume processes of the type (Hovd et al., 1997)

$$\mathbf{G(s)} = \mathbf{W_0}\mathbf{\Sigma(s)}\mathbf{V_0^T} \tag{15}$$

where $\mathbf{W}_0$ and $\mathbf{V}_0$ are independent of frequency and the frequency-dependent matrix $\mathbf{\Sigma(s)}$ is diagonal, then Eq. (14) also holds for non-steady-state data.

We conclude that, assuming a model with frequency-independent directionality (Eq. 15), and an identification experiment using uncorrelated inputs, we can employ PCA to extract the gain directions from the outputs. In practice, we can expect a slow high-gain response in the first principal component and a faster low-gain response in the second principal component, which are straightforward to identify with e.g. first-order models.

2.4 Identification Using Output Rotation

Next, we suggested a method for identification of ill-conditioned systems that uses output rotation and the example models G_{62} (3) and G_{51} (5). We continue the discussion with two-input-two-output processes, but the concept can be extended to processes with more inputs and outputs.

We start with design of input excitation. For ill-conditioned processes it is common to design input excitation such that the low gain direction is sufficiently perturbed. This can only be done if an estimate of the steady-state gain is available. At this point, however, we do not assume any knowledge of the process so at least the initial experiment is done using uncorrelated input excitation. If needed, the identification experiment is extended with excitation of the process in the low gain direction, which is often necessary if the low gain direction is hidden by noise and disturbances. This is discussed later.

Initially any uncorrelated input excitation method may be used (sequential or simultaneous steps or PRBS or other). After the identification experiment, with the input-output data matrices collected, we start with output scaling and rotation. With PCA it is common practice to scale each output signal to obtain zero mean and unity variance. Applying PCA to the outputs, we obtain the rotated outputs, i.e. the principal components $\mathbf{T}$.

With rotated outputs we identify the high gain direction first, i.e. we identify a model from inputs to the first principal component (t_1). Applying Eq. (14) and (15) on models G_{62} and G_{51} we can expect a first-order response governed by time constant T_1 in the high-gain direction, so we start by identifying the parameters k_{v1}, k_{v2} and T_1 of the model

$$t_1(s) = \frac{k_{v1}u_1(s) + k_{v2}u_2(s)}{T_1 s + 1} \tag{16}$$

Here any system identification method can be used, but in the examples below we use least-squares identification of ARX models. With k_{v1}, and k_{v2} identified, we can determine the matrix $\mathbf{V}$ assuming that the low gain direction is orthogonal to the high gain direction. We can, for example, select

$$\mathbf{V} = \begin{pmatrix} k_{v1} & k_{v1} \\ k_{v2} & -k_{v2} \end{pmatrix} \tag{17}$$

With $\mathbf{V}$ known, the low gain direction identification reduces to identification from input

$$u_{lg} = k_{v1}u_1 - k_{v2}u_2 \tag{18}$$

to second principal component t_2. For model G_{62} (Eq. 3) we identify parameters k_2 and T_2 of the single-input-single-output model

$$t_2(s) = \frac{k_2}{T_2 s + 1} u_{lg}(s) \tag{19}$$

At this point we evaluate the identification result. Commonly, the high gain direction (Eq. 16) is easy to identify, but the model fit in the low-gain direction (Eq. 19) is worse. Therefore, the low-gain direction fit is a clear indication of identification success. When the low gain fit is poor, we need to continue with input excitation in the low-gain direction (Eq. 18) and re-identify the low gain.

Note that there is no need to modify output rotation or high-gain identification when we continue with process excitation in the low gain direction. All we need to do is to re-identify the low gain direction. Again, model fit in low gain direction is a good measure of success.

The identification method is summarized in Table 1 for a 2×2 system.

Table 1. Summary of identification using output rotation

Step	Description
1	Perform a standard identification experiment consisting of input excitation and data collection. At this point the inputs must be uncorrelated, but otherwise any excitation method can be used (step, PRBS, etc.).
2	Make a PCA analysis to obtain the first and second principal components of the outputs. PCA also gives the output rotation matrix $\mathbf{W}$.
3	Identify a model from inputs to first principal component (Eq. 16).
4	Identify the input rotation matrix $\mathbf{V}$ (Eq. 17).
5	Identify a model from low-gain input direction (Eq. 18) to second principal component (Eq. 19).
6	Evaluate the quality of the identified second principal component.
7	If evaluation result in step 6 was good, model is identified, otherwise continue with excitation in low gain direction and go to step 5.

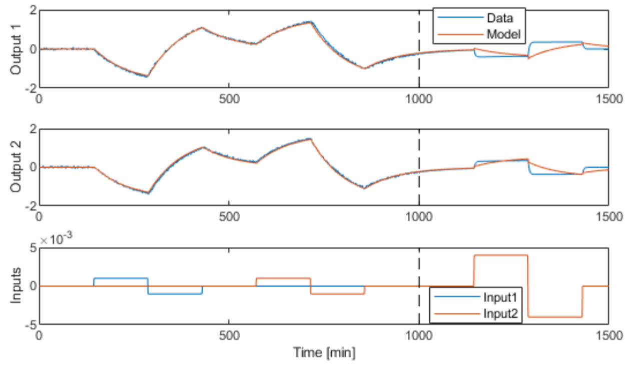

Fig. 1. Identification of the Heat Exchanger example ($t < 1000$), and validation in the difficult low gain direction ($t > 1000$)

2.5 *Case Example 1: A Linear Heat Exchanger Model*

Consider the heat exchanger model discussed by Jacobsen and Skogestad (1994). The model is

$$G(s) = \frac{89.243}{(T_1 s + 1)(T_2 s + 1)} \begin{pmatrix} -21(T_3 s + 1) & 20 \\ -20 & 21(T_3 s + 1) \end{pmatrix} \tag{20}$$

with $T_1 = 100$, $T_2 = 2.439$, and $T_3 = 4.762$. This model is ill-conditioned with a condition number 41. There is a clear difference in the dynamics of the high and low gain directions, indicated by time constants T_1 and T_2.

To demonstrate the difficulties of identifying this model, and to illustrate output rotation, we simulated the system, added some noise and disturbances, back-identified the model from the simulated data, and evaluated the results. Models were simulated using discretized models with sampling time $T_s = 1$.

Model fit was calculated from average ($\bar{y}$), estimated ($\hat{y}_i$) and measured (y_i) outputs as (Ghosh, 2016)

$$F_p = 1 - \frac{\sum_i (\hat{y}_i - y_i)^2}{\sum_i (y_i - \bar{y})^2} \tag{21}$$

For multi-variable models we use Eq.(21) to calculate the fit for each variable but report the average fit, unless otherwise stated.

First we used a traditional system identification method to obtain the parameters of model G_{106} (Eq. 2) using ARX models and standard least-squares identification.

The simulated responses of the Heat Exchanger (Eq. 20) and for the identified model are shown in Fig. 1. As expected, we get a good model fit for the test data (left part of the figure, $t < 1000$). However, when we validate the model with excitation in the tricky low gain direction (right part, $t > 1000$) we notice that the low gain has been poorly identified.

The reason for modeling failure is that it is difficult to properly identify all parameters of model (2) with noise in the outputs.

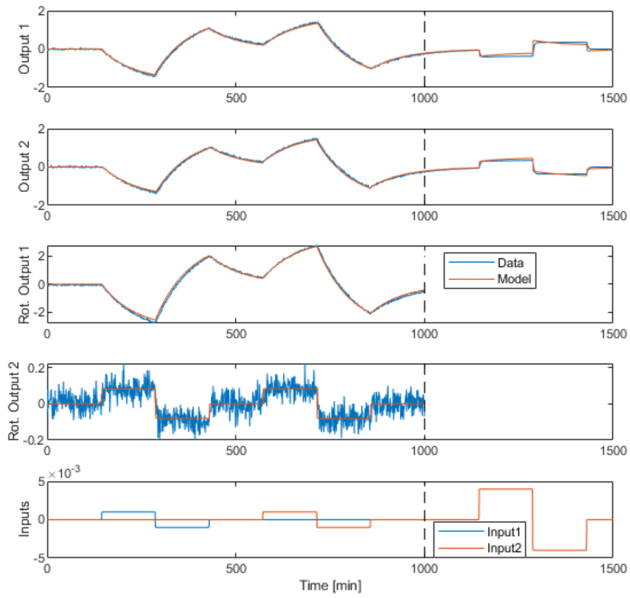

Fig. 2. Same as Fig. 1 but with identification in the rotated domain.

Next we demonstrate how the same identification task is done using model G_{62} (Eq. 3) and output rotation. We rotated the outputs using standard PCA (with standard deviation scaling) and identified the process from inputs to rotated outputs. The trends, both measured and rotated outputs are illustrated in Fig. 2. Above are shown the two outputs, and third from above is the high gain direction (first principal component), which is well identified. Fourth trend from above is the low-gain direction (second principal component) which is clearly more difficult to identify. The low gain direction is almost hidden in noise because the low gain is only slightly perturbed. Still, both high and low gain directions can be identified, and we get a good model fit also in the validation part ($t > 1000$).

The heat exchanger example demonstrates some advantages with the suggested method. With traditional identification, which identifies the process from physical inputs to physical outputs, the model fit looks good even though it is not. With the suggested method, however, we get a realistic impression of the identification quality, seen in the low-gain fit. A clear advantage with rotated outputs is that we have fewer parameters at the identification step. In this case the identification results are also better, considering the validation results.

We did a large number of simulation experiments with model (20), and fitted it to the models G_{106}, G_{62}, and G_{51}, with different input/output disturbances and types (from white noise to random walk). Fig. 3 illustrates the model fit as a function of noise level (with white noise added to the outputs). Fig. 4 illustrates the impact of input disturbances on the identification result. For the input disturbances we used random walk noise, as disturbances are usually auto-correlated.

From Fig. 3 and 4 we conclude that G_{106} is extremely sensitive to output noise and that there are practically no significant difference between models G_{62} and G_{51}. This result suggests that we should neglect the low gain

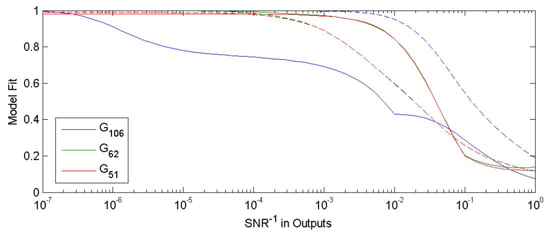

Fig. 3. Model fit obtained from identification of the heat exchanger example with white noise added to the outputs, and noise level increasing from left to right. The trends show model fit for validation experiments (solid lines) and test experiments (dashed lines) of the models G_{106}, G_{62}, and G_{51}.

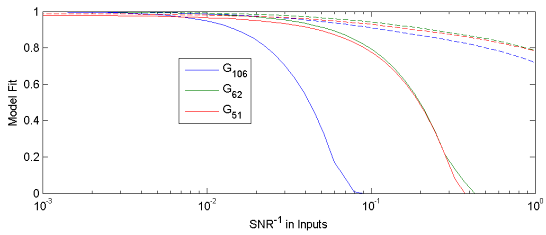

Fig. 4. Same as Fig. 3 but with random walk noise added to the inputs.

time constant T_2 when it is clearly smaller than the time constant in the high-gain direction (in this case $T_1 = 100$, $T_2 = 2.439$).

2.6 Case Example 2: A Non-Linear Distillation Column

In this section we test the suggested method on a simulated distillation column model, "Column A" discussed by Skogestad and Morari (1988) and Skogestad and Postlethwaite (2007). The column has 40 theoretical stages and separates a binary mixture into products of 99% purity, and it captures the main effects important for dynamics and control. We used the Matlab implementation of the model, which is available on the internet (Skogestad, 1997).

The Column A model uses feed flow and feed composition as inputs, so it is easy to add disturbances to make realistic experiments. Here we used random walk disturbances in the feed flow and composition. To speed up the simulations, we modified the disturbances once every 60$^{\text{th}}$ minute.

Fig. 5 shows an identification experiment of the non-linear distillation column. The first part of the experiment, i.e. time up to 5000 min, is evaluated first. In this part the high-gain direction (3$^{\text{rd}}$ plot from above, Eq. 16) is well identified but we are unable to identify the low gain direction (4$^{\text{th}}$ plot from above, Eq. 19). The low-gain excitation is weak, and only some perturbation resulting from model non-linearities are seen in the trend. Therefore it is evident that the low gain direction can not be identified based on the first 5000 minutes.

At time instant $t = 5000$, a decision to continue the identification experiment by excitation of process in the low gain direction (Eq. 18) was made. In Fig. 5, for time $t > 5000$, is shown that this excitation enables

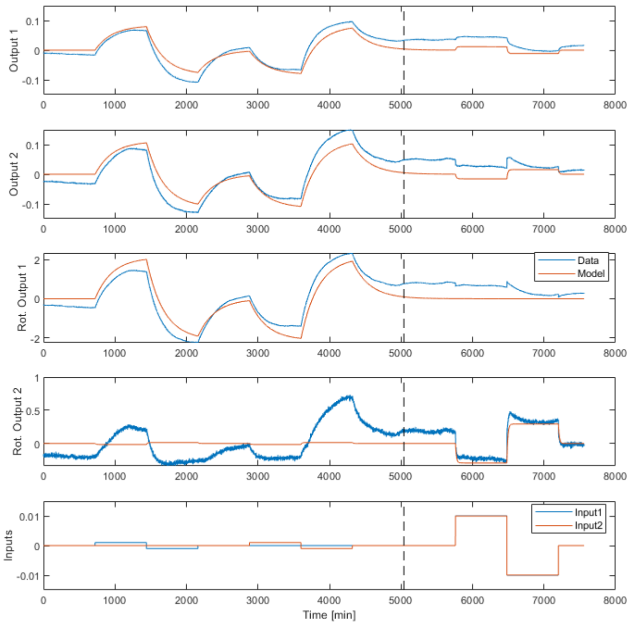

Fig. 5. Identification of the Column A model.

identification of the low gain direction (4^{th} plot from above, $t > 5000$). Hence, the parameters of model G_{62} (Eq. 3) could be successfully identified.

2.7 Summary and Conclusions

We have suggested a new method for identification of ill-conditioned processes. The main idea is to identify the output rotation matrix from output data using principal component analysis (PCA) before the actual identification step. As a result, the identification step simplifies from identification of high-order MIMO models in one step to identification of first-order models one output at a time. Simple ARX identification methods can be used.

The suggested concept has many advantages important for industrial applications. We get a reliable assessment of identified model quality. We can capture the directionality of the process, both gain and dynamics, which is crucial when the model is used for control purposes. Still, compared to traditional identification methods, we can reduce the number of parameters and states in the models. Simple least-squares identification of ARX models one output at a time can be used, so only lightweight tools are needed in the calculations. By identifying the process in directions important for control, it is easier to ensure integral controllability. The main drawback of the suggested method is that both SVD and PCA depend on scaling. Scaling to unit variance often works well but not always. If we notice large overshoots in the second principal component, it is an indication that we should modify scaling.

Future plans include extending the concept from open-loop to closed-loop identification (Friman, 2020), and investigating how the simple models (in particular the single state model G_{51}) perform in model-based control of high-purity distillation columns.

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