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Sensor Configuration Problem: Application to a Membrane Separation Unit ⋆

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Abstract: For high performance model based control applications the state and parameter estimation algorithms are essential. Furthermore the accuracy of the resulting estimates highly depends on what is being measured. In this work we address the output channel selection problem by making use of the degree of observability measures defined by the observability gramians of the associated system and possible different sensor configurations. The observability gramians for large scale and nonlinear first principle models are difficult to compute. Instead the data based approximations, the empirical observability gramians, are constructed. The degree of observability measures are used for comparing the spectral properties of the observability gramians to decide the sensor configuration. The output channel selection procedure is applied to an industrial membrane filtration system.

Keywords: Sensors, Decision making, Optimal estimation, Identifiability, Observability gramian, Degree of observability, Output covariance matrix.

1. INTRODUCTION

The motivation of using first principle models for online model based operations like process control and monitoring has led to several research directions in the systems and control area. Some of these directions focus on overcoming the computational complexity either by developing model reduction techniques or computationally efficient optimization and simulation algorithms. However, the online use of first principle models is also hampered by the degradation of model accuracy over time (catalyst deactivation, fouling etc.). This is, in fact, a general concern for any model type. Some of the recent research has been in the area of maintaining the accuracy of these models since the performance of any model based application is affected by the quality of the model (Kravaris et al. (2013)).

A research topic which has been investigated to improve and maintain model accuracy is the area of parameter estimation (Kravaris et al. (2013); Lund and Foss (2008); Tarantola (2005)). Parameter estimation problems are concerned with obtaining accurate estimates of unknown or varying parameters by using the measured input-output data. These works include parameter estimation algorithms, observer design techniques and also methods to decide which parameters to estimate (Lund and Foss (2008); Li et al. (2004)). Similar to these the quality of the estimation results depend on what is being measured. In this work, we address the optimal sensor configuration (OSC) problem for state and parameter estimation purposes in order to achieve high model accuracy and improved maintenance.

The problem of state and parameter estimation requires the concepts of observability and identifiability, which indicate whether the initial state or parameters can be uniquely distinguished from the input and output measurements. However determining whether the system is observable or not, is not enough to decide what to measure. The OSC problem might require comparison of different measurement channel configurations with respect to the resulting variance of the estimates or the numerical reliability of the estimates, while all of the output configurations might render the system to be observable (Sumana and Venkateswarlu (2009); Van den Berg et al. (2000)). To this end, we use the *degree of observability measures* to indicate how informative sensors are. Many of these measures are based on the spectral properties of the observability gramian (Müller and Weber (1972)). These different measures on the observability gramian may lead to different 'optimal' sensor configurations (with respect to (w.r.t.) different measures). Thus, a multi-objective optimization scheme could be utilized to solve the OSC problem (Singh and Hahn (2006)).

In order to use the degree of observability measures for the OSC problem, we need to construct the observability gramian. This matrix reflects the influence of the states on the measurements and hence provides a description of the state-output behaviour of a system (Sumana and Venkateswarlu (2009)). In literature, many of the studies consider the linear time-invariant (LTI) or linear time-varying approximations of the complex system for deciding which signals to measure. This is due to the ease of solving the OSC problem with the observability gramian (Van den Berg et al. (2000)), or the observability matrix (Tali-Maamar et al. (1994)), or the Hautus' test, (Waldraff et al. (1998)). However, all of these methods are only valid for linear systems. One can make use of the differential-geometric techniques (Nijmeijer (1982)) or the tools from lie algebra (Brockett (1973)) for addressing the observability property of nonlinear systems. For large scale systems, these techniques are almost impossible to apply, since the computational demand

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required to solve the problem is tremendous (Scherpen and Gray (2000)). Many other algorithms are developed to address the OSC problem in relation to the estimation quality. For example, metrics on the error covariance matrix of the implemented Kalman filter are developed in Omatu et al. (1978) and Kumar and Seinfeld (1978). Although the connection between the Fisher information matrix and the gramian is known for a long time, (Bellman and Åström (1970)), the analytic relations for the bounds on the spectral properties of the state estimation covariance matrix derived from the observability gramian is missing. A discussion on these bounds can be found in (Huxel and Bishop, 2009, §4.3).

Recently data-based methods are introduced to approximate the controllability and observability gramians of nonlinear systems with empirical counterparts (Lall et al. (2002)). These (covariance) matrices are used for the balanced truncation approach in the model reduction problems for nonlinear systems (Hahn et al. (2003)). These type of algorithms suffer from the number of experiments/simulations that are needed to be done. Generally one needs to conduct many simulations to include the effect of nonlinear behaviour into the empirical gramian matrix. However once the data is gathered, the effect of the states (and consequently the parameters) can be observed in the gramian matrix which is obtained only from the data. As indicated in Singh and Hahn (2005a), combining the computational ease of the calculating output covariance matrix with the established measures for OSC problem that are valid for linear systems is a big step for solving the OSC problem for nonlinear systems.

In this paper we present a procedure to decide upon the output measurement channels of a complex system, represented with unstable nonlinear differential algebraic equations (DAEs), to estimate the parameters and states effectively. The decision is made by using the measures cast on the observability gramians of the system. Due to the nonlinearities and instabilities, the conventional observability gramians are not available. Instead, we make use of the empirical observability gramians. Until now the empirical observability gramians are constructed for stable nonlinear systems by utilizing the steady state operating values. Our contribution is to define the empirical observability gramians for unstable systems through the nominal trajectories of the unstable states. There is no theoretical limitation to extend the definition of empirical gramian by using nominal trajectories, hence the approximation is converging to the exact (finite time) gramian. The effectiveness of selected sensor channels are compared with respect to the degree of observability measures cast on the empirical gramian, thus the measurement channel decision can be made in a rigorous manner.

The structure of the paper is as follows. In Section 2 we state the mathematical problem by introducing observability and identifiability properties, the (empirical) observability gramian and the measures on the degree of observability. In Section 3 we apply these concepts to an unstable DAE system, which represents a simplified industrial membrane filtration process. In Section 4 conclusions are presented.

2. PROBLEM FORMULATION AND BACKGROUND INFORMATION

The OSC problem is connected to the effect of the states and parameters to the output measurements, which can be tracked with the spectral properties of the observability gramian. One important spectral property of the observability gramian, i.e., its positive definiteness, is also connected to the observability (and identifiability) concept, from which we start our discussion. For this purpose we consider a DAE system in the form of (1)

$$\Sigma : \begin{cases} \dot{x}(t) = f_d(x(t), z(t), p, u(t)), \\ 0 = f_a(x(t), z(t), p, u(t)), \\ y_i(t) = h_i(x(t), z(t), p, u(t)), \end{cases} \tag{1}$$

where $x(t) \in \mathbb{R}^{n_x}$ $(t \in \mathbb{R}_{[0,t_f]})$, is the differential state, $z(t) \in \mathbb{R}^{n_z}$ is the algebraic state, $p \in \mathscr{P} \subseteq \mathbb{R}^{n_p}$ is the (unknown) parameter vector associated with the model, $u : [0,t_f] \to \mathbb{R}^{n_u}$ is the input and $y_i(t) \in \mathbb{R}^{n_{y_i}}$ is the measured output for the i^{th} possible output configuration, in which $i \in \mathscr{I} := \{1, 2, \ldots, n_i\}$ and h_i is the associated sensor configuration, being an element of the set of possible measurement channels $\mathscr{C}$. Our task is to decide the 'best' sensor configuration h_i to improve the state and parameter estimation accuracy. The initial condition at $t = t_0$ of Σ is denoted with x_0. It is assumed that the functions f_d and f_a are analytic, the Jacobian $\partial f_a / \partial z$ is invertible at all points (x, z, u) and the differentiation index of DAE model is equal to one, hence there exists a linear approximation Σ_{lin} on the trajectory $(\bar{x}(t), \bar{z}(t), \bar{u}(t))$ with deviation variables $\delta x, \delta u$, i.e.,

$$\Sigma_{lin} : \begin{cases} \delta\dot{x}(t) = A(t,p)\delta x(t) + B(t,p)\delta u(t) + g(t,p), \\ \delta y_i(t) = C_i(t,p)\delta x(t) + D_i(t,p)\delta u(t) \end{cases}$$

The observability and identifiability properties play a crucial role in state and parameter estimation problems to result in correct estimates. We start with the observability concept.

Definition 2.1. The model Σ, with known parameters p and input $u(t)$, is *observable* if the initial state x_0 can be uniquely determined from the inputs and outputs $u(t), y(t)$ for $t \in \mathbb{R}_{[t_0,t_f]}$;

$$\exists u(t), \exists p, \forall x_0^1, x_0^2, t \in \mathbb{R}_{[t_0,t_f]} : y_i^1(t) = y_i^2(t) \implies x_0^1 = x_0^2,$$

where $y_i^1(t)$ and $y_i^2(t)$ are the output values obtained from input $u(t)$ and the initial conditions x_0^1 and x_0^2, respectively.

One of the main tools for analyzing observability is the observability gramian, $W_o : \mathbb{R}_{\geq 0} \times \mathbb{R}_{>0} \to \mathbb{R}^{n_x \times n_x}$. For the linearized model Σ_{lin} and time instants $t_f > t_0 \geq 0$, $W_o^i(t_0, t_f)$ is defined as

$$W_o^i(t_0,t_f) := \int_{t_0}^{t_f} \psi_i^T(p,\tau,t_0)\psi_i(p,\tau,t_0)d\tau. \tag{2}$$

where $\psi_i(p,t_1,t_0) = C_i\phi(p,t_1,t_0)$ and $\phi(p,t_1,t_0)$ is the state transition matrix from t_0 to t_1. Observe that $\psi_i(p,t_1,t_0) = \partial(\delta y_i(t_1))/\partial(\delta x_0)$, hence $W_o^i(t_0,t_f)$ summarizes the effects on the deviated output δy by the perturbations on the initial state δx_0.

For linear deterministic systems, the observability gramian is full rank if and only if the system is observable hence the states are uniquely reconstructible. Furthermore, for nonlinear systems with differentiable function f_d, the nonsingular observability gramian implies local observability around x_0.

Now we define the identifiability concept which relates the effects of parameter variations to the output measurements.

Definition 2.2. (Grewal and Glover (1976)) The parameterized model Σ with a set of parameters $p \in \mathscr{P}$ is locally identifiable if the parameters are distinguishable from each other given the initial state x_0, the inputs $u(t)$ and the outputs $y_i(t)$ for $t \in \mathbb{R}_{[0,t_f]}$;

$$\begin{aligned} &\exists x_0,\ \exists u(t), t \in \mathbb{R}_{[0,t_f]},\ \ \forall p_1, p_2 \in \mathscr{P} : \\ &\qquad\qquad y_i^1(t) = y_i^2(t) \implies p_1 = p_2. \end{aligned} \tag{3}$$

where $y_i^1(t)$ and $y_i^2(t)$ are the output values obtained from input $u(t)$, the initial condition x_0 and the parameters p_1 and p_2.

The identifiability property guarantees that any deviation in the parameters eventually effect the outputs on the operating trajectory. One general way of checking identifiability, given input and initial condition, is by constructing the parameter-to-output sensitivity matrix, i.e., $\mathscr{W}_p^i(t) := \partial y_i(t)/\partial p$. This matrix is connected with the observability gramian of the (new) system constructed with the parameters, i.e., p in Eq.(1), augmented as new states, i.e., $\dot{p} = 0$. Then the observability matrix of the augmented system contains the information deduced from the parameter-to-output sensitivity matrix, i.e.,

$$\bar{W}_o^i(0,t_f) = \begin{bmatrix} W_o^{i^{xx}} & W_o^{i^{xp}} \\ W_o^{i^{px}} & W_o^{i^{pp}} \end{bmatrix} = \int_{t_0}^{t_f} \begin{bmatrix} \left(\frac{\partial y_i}{\partial x_0}\right)^T \frac{\partial y_i}{\partial x_0} & \left(\frac{\partial y_i}{\partial p}\right)^T \frac{\partial y_i}{\partial x_0} \\ \left(\frac{\partial y_i}{\partial x_0}\right)^T \frac{\partial y_i}{\partial p} & \left(\frac{\partial y_i}{\partial p}\right)^T \frac{\partial y_i}{\partial p} \end{bmatrix} dt.$$

Under this construction the parameter identification problem boils down to the problem of the observability of states of the augmented system.

Since the observability gramian is utilized for both the state and parameter estimation problems, we consider methods that construct the gramian for large scale and nonlinear models with relatively low computational complexity. For nonlinear systems the construction of the observability gramian does not follow from the linear case trivially. One can overcome this problem by the empirical observability gramian. This matrix is constructed via the output measurements which are obtained from (nominal and perturbed) initial states (and initial parameters) by calculating the covariance matrix of the output measurements. The empirical observability covariance matrix for system (1) is calculated as (Singh and Hahn (2005b));

$$\hat{W}_o^i(t_0,t_f) := \sum_{l=1}^{r}\sum_{m=1}^{s} \frac{1}{r}\frac{1}{s}\frac{1}{c_m^2}\int_{t_0}^{t_f} T_l \Psi^{lm}(t,i) T_l^T\, dt, \tag{4a}$$

where r and s are the cardinalities of the sets of perturbation directions (T^{r,n_x}) and magnitudes (M);

$$T^{r,n_x} = \{T_1,\dots,T_r; T_l \in \mathbb{R}^{n_x\times n_x}, T_l^T T_l = I, l = 1,\dots,r\}, \tag{4b}$$
$$M = \{c_1,\dots,c_s; c_s \in \mathbb{R}, c_m > 0, m = 1,\dots,s\}, \tag{4c}$$

and the $(jk)^{\text{th}}$ element of the matrix $\Psi^{lm}(t,i) \in \mathbb{R}^{n_x\times n_x}$ is defined as

$$\Psi_{jk}^{lm}(t,i)(t) = (y_i^{jlm}(t) - \bar{y}_i(t))^T (y_i^{klm}(t) - \bar{y}_i(t)),$$

with $y_i^{jlm}(t)$ being the output of the system corresponding to the initial condition $x^{jlm}(0) = c_m T_l e_j + \bar{x}_0$, e_j being the j^{th} basis direction in $\mathbb{R}^{n_x}$ and $\bar{y}_i(t)$ is the nominal-unperturbed output of the system initiated from the nominal state $\bar{x}_0$. All of the output trajectories, $y_i^{jlm}(t)$ and $\bar{y}_i(t)$, are steered with input $\bar{u}(t), t \in [0,t_f]$. For stable systems one can use the steady state values of states and outputs, see, e.g., Singh and Hahn (2005a). However for an unstable system, since no steady state values exist, we propose that one should take the $\bar{y}_i$ values as the nominal (unperturbed) trajectory while calculating the empirical gramian. In this case observe that $y_i^{jlm} \approx \bar{y}_i + \delta y_i^{jlm}$, hence $\Psi_{jk}^{lm}(t,i) = (e_j^T T_l^T c_m)\psi_i^T(p,t,t_0)\psi_i(p,t,t_0)c_m T_l e_k$ (since $\delta u(t) = 0$ for $t \in [t_0,t_f]$), which yields to true observability gramian after evaluating the integral and the sums in Eq. (4a). Hence if the model equations Eq. (1) are sufficiently smooth and the linear approximation for perturbations defined by T_l and c_m is valid, then the empirical observability gramian converges to the true observability gramian. Thus, from a system theoretical point of view, both the theoretical and computational problems induced by nonlinearities or instabilities are discarded with the empirical observability gramian approximation.

The operating region is highly effective on the calculated gramian which should reflect the nonlinear behavior in the covariance matrix. The approximation quality of the empirical observability gramian to the real observability gramian of the system is determined by the selection of sets T^{r,n_x} and M. The set of perturbations T^{r,n_x} should be selected such that $c_m T_l e_j$ terms excite the nominal initial state $\bar{x}_0$ in all of the directions spanning the state space, both the positive and negative directions to approximate $\partial y_i(t)/\partial x_0$; while the perturbation magnitudes c_m should be selected wisely to capture the whole region of interest by adjusting the magnitudes of the elements of M, see e.g., Singh and Hahn (2005a).

In practice, the initial state might be difficult to reconstruct from data, if the observability gramian is ill-conditioned. To briefly elaborate, consider the gramian based state estimates $\delta\hat{x}(t)$ for model Σ_{lin} with $\delta u(t) = 0, t \in [t_0,t_f]$,

$$\delta\hat{x}(\tau) = W_o^{i^{-1}}(t_0,\tau)\int_{t_0}^{\tau}\phi^T(p,s,t_0)C_i^T\delta y_i(s)ds,\ \tau \in (t_0,t_f].$$

If the observability gramian is ill-conditioned, this will cause poor results for the estimates. In this paper this issue is taken into account with the degree of observability measures. These measures are cast on the (true or empirical) observability gramian to compare different output channels with respect to the informativity of the measured signals. Several of these measures are listed below, for the set of possible output channels $\mathscr{C}$.

Eigenvalues: The minimum eigenvalue of the observability gramian indicates how close the system is to becoming unobservable, hence higher values of the smallest eigenvalue imply a greater degree of observability measure, i.e.,

$$\mu_1 := \max_{h_i\in\mathscr{C}} \arg\min_{\lambda}\{\lambda(W_o^i(t_0,t_f))\}.$$

However the eigenvalue measure does not reflect the effect of perturbations in other directions than the eigenvector associated with the minimal eigenvalue. Hence in general it is difficult to assess the overall performance through the eigenvalue measure.

Trace: The second measure compares the trace of the observability gramians w.r.t. different sensor selections, i.e.,

$$\mu_2 := \max_{h_i\in\mathscr{C}} \text{trace}(W_o^i(t_0,t_f)) = \max_{h_i\in\mathscr{C}}\left\{\sum_{j=1}^{n}\lambda_j(W_o^i(t_0,t_f))\right\}.$$

The trace is the sum of eigenvalues, hence representing the maximum effect on the output w.r.t the perturbations in all directions. It is observed that (Singh and Hahn (2005a)) for OSC problem with estimation purposes, the measure μ_2 yields better results compared to the other measures defined here.

Determinant: The third measure is the determinant of the observability gramian. A larger determinant of $W_o^i(t_0,t_f)$ shows that at least one eigenvalue is larger compared to the other sensor configurations. Therefore the largest determinant case of the gramians constructed for different sensor selections corresponds to a better output channel configuration, i.e.,

$$\mu_3 := \max_{h_i\in\mathscr{C}} \det(W_o^i(t_0,t_f))^{\frac{1}{n}}.$$

The determinant measure is numerically problematic and varies with a high dependence on the elements of the gramian matrix, thus depends heavily on the selection of T^{r,n_x} and M matrices for empirical observability gramian calculation.

Condition number: For state estimation quality, one needs to consider the maximum and minimum singular values and associated directions of the observability gramian. Another method that can be utilized for the OSC problem is the condition number of the gramian, which is defined as

$$\kappa(W_o^i(t_0,t_f)) := \frac{\sigma_{max}(W_o^i(t_0,t_f))}{\sigma_{min}(W_o^i(t_0,t_f))}.$$

This method can be viewed as a tool for analyzing the sensitivity of the observability property w.r.t. different measurement channels (Dochain et al. (1997)). A small valued $\kappa(W_o^i(t_0,t_f))$ implies that the magnitude difference between $\lambda_{max}(W_o^i(t_0,t_f))$ and $\lambda_{min}(W_o^i(t_0,t_f))$ is small, hence a less ill-conditioned observability gramian. This improves the estimation quality, hence this measure minimizes the condition number, i.e.,

$$\mu_4 := \min_{h_i \in \mathscr{C}} \kappa(W_o^i(t_0,t_f)) = \min_{h_i \in \mathscr{C}} \left\{ \log\left(\frac{\sigma_{max}(W_o^i(t_0,t_f))}{\sigma_{min}(W_o^i(t_0,t_f))} \right) \right\}.$$

Apart from these, one can make use of the spectral radius or the near singularity measures as indicated in Singh and Hahn (2005a).

Remark 1. Since the analytic relations between the spectral properties of observability gramian and state (or parameter) estimation covariance matrix are missing, there is no straightforward way to select the OSC minimizing estimation error variance through the above mentioned measures. These measures are only used as an indicator for the selection procedure.

3. SIMULATION EXAMPLE OF A DAE SYSTEM

3.1 Whey Ultrafiltration Membrane Model

Whey ultrafiltration (UF) membrane systems are pressure driven separation units, where the proteins in whey are filtrated away from other components, such as fats or salts. These system are represented with unstable, nonlinear DAE models (Guadix et al. (2004)). The differential equations model the membrane resistance which is always increasing due to the fouling effect. In this study the membrane set-up consists of two membrane stages and a circulation pump, to provide the desired pressure levels, which are connected in series to each other. There are two outlet streams, and hence output channels, of membrane stacks, the permeate and the retentate streams. We provide a simple schematic of a membrane system with two stages in Figure 1. The mathematical model of the membrane system is taken from Guadix et al. (2004) as

$$\begin{aligned}
F_f^j &= F_r^j + F_p^j, \quad & F_f^j C_f^j &= F_r^j C_r^j, \\
F_p^j &= A J^j, \quad & J^j &= \frac{\Delta P^j}{R^j}, \\
\Delta P^j &= P_{in}^j - \frac{1}{2}\delta P^j - P_{atm}, \quad & \dot{R}^j &= \alpha (\Delta P^j)^\beta J^j C_r^j, \\
P_{in}^2 &= P_r^1 = P_{in}^1 - \delta P^1, \quad & j &= 1,2,
\end{aligned} \tag{5}$$

where $j = 1,2$ is the index over two membrane stacks, the feed, retentate and permeate mass flows are denoted with F_f^j, F_r^j, F_p^j,

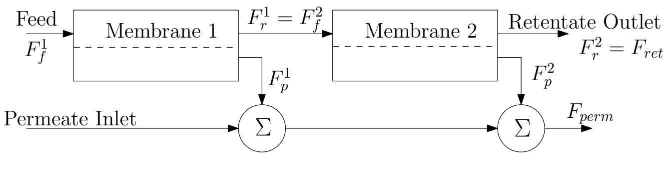

Fig. 1. The two membrane stacks system.

respectively, C_f^j and C_r^j denote the concentrations of feed and retentate stream, J^j is the mass flux, and R^j is the membrane resistance. The state and parameter vectors are defined as

$$x = \begin{bmatrix} R^1 & R^2 \end{bmatrix}^T, \qquad p = \begin{bmatrix} \alpha^1 & \alpha^2 \end{bmatrix}^T.$$

We simplify the model in Guadix et al. (2004) by not considering osmotic pressure since for UF purposes these terms are not effective during the operation. The parameter values, initial state and operating conditions are tabulated in Table 1. The operating conditions are selected in such a way that the performance outputs, F_r^2, C_r^2, are kept in acceptable levels with the linear increase of the pressure, the input u. Furthermore, the initial conditions are determined through the geometry (pore size/density etc.) and operating conditions of the membranes. Lastly, we assume that the membranes foul at $t_f = 10$, thus the process execution is interrupted.

Area of membrane stack (m^2)	A	74.0350
Pressure drop over membrane (Pa)	δP_i	100
Atmospheric pressure (Pa)	P_{atm}	101.3
Fouling parameter 1 (-)	α	0.0005
Fouling parameter 2 (-)	β	0.5
Inlet pressure (Pa)	$P_{in}^1(t)$	$10^3(1/2 + t/t_f)$
Inlet mass flow (kg/h)	F_1^1	5000
Inlet protein concentration (kg/L)	C_1^1	5
Initial membrane resistance (-)	$R_1(0) = R_2(0)$	15

Table 1. Nominal parameter values and operating conditions.

3.2 State Estimation with Empirical Observability Gramian

The possible measurement channels are taken as the mass flows at the retentate and permeate ports. There are seven different output channels which are characterized as

$$y_i = C_i^T \begin{bmatrix} F_{perm} \\ F_{ret} \\ F_r^1 \end{bmatrix},$$

where the output channels C_i are the elements of the set $\mathscr{C}$;

$$\mathscr{C} = \left\{ \begin{bmatrix}1\\0\\0\end{bmatrix}, \begin{bmatrix}0\\1\\0\end{bmatrix}, \begin{bmatrix}0\\0\\1\end{bmatrix}, \begin{bmatrix}1\\1\\0\end{bmatrix}, \begin{bmatrix}0\\1\\1\end{bmatrix}, \begin{bmatrix}1\\0\\1\end{bmatrix}, \begin{bmatrix}1\\1\\1\end{bmatrix} \right\}. \tag{6}$$

The F_{perm}, F_{ret} and F_r^1 are visualized in Figure 1 and given as

$$\begin{aligned}
F_{perm} &= F_p^1 + F_p^2 + F_{perm}^{inlet}, \; F_{perm}^{inlet}(t) = 0, \\
F_{ret} &= F_r^2.
\end{aligned} \tag{7}$$

For the given set of possible output configurations, we calculate the empirical observability gramian with Eq. (4a) to calculate the degree of observability measures μ_k. We select the perturbation directions as the positive and negative directions in the state space and the perturbation magnitudes are less then 10% of the initial conditions (see Table 1), i.e.,

$$\begin{aligned}
T^{2,2} &= \{I_2, \; -I_2\}, \\
M &= \{1.5, \; 1, \; 0.75, \; 0.5, \; 0.25\}.
\end{aligned}$$

The degree of observability measure results for membrane system and empirical observability gramian are visualized in Figure 2. From these results we observe that output channel cases 3-5-6 and 7 are providing sufficient information regarding the states of the system, whereas the case 7, measuring the sum of three variables, is the optimal choice for the state estimation purposes. This is due to the output measurements that contain

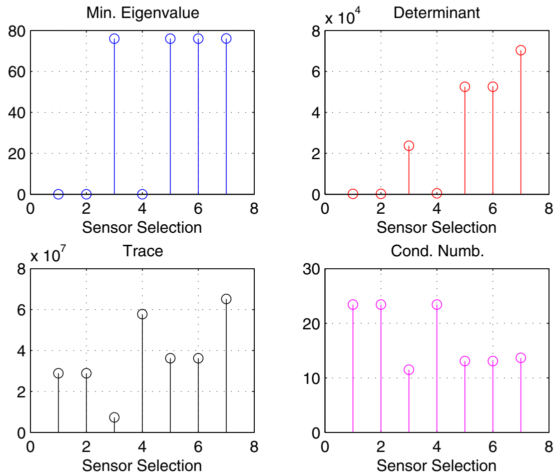

Fig. 2. Degree of observability measure results obtained for two membrane stack system for state estimation problem.

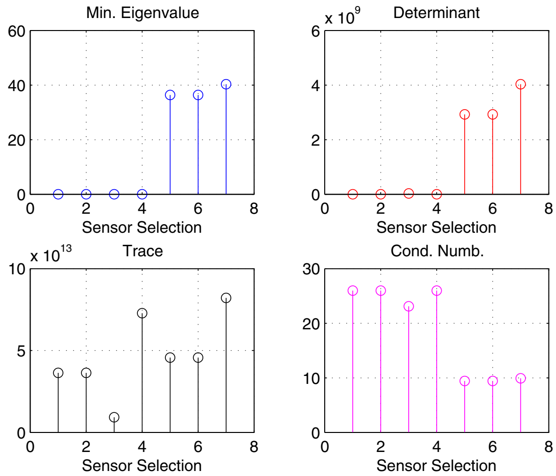

Fig. 3. Degree of observability measure results obtained for two membrane stack system for state and parameter estimation problem.

the largest amount of information. Case 5 and 6 represent the instances measuring the sum of retentate mass flow of first membrane with the outlet permeate or retentate streams, respectively. Observe that all of the degree of observability measures are equal to each other in these two output configuration cases due to the model equation

$$F_f^i = F_r^i + F_p^i,$$

where F_f^1 is assumed to be known. Furthermore, measuring the two streams together causes the system to become unobservable, as seen from the case 4. The optimal sensor selection results correspond to the industrial implementations, where the mass flows of each membrane stack are tracked.

3.3 Parameter Estimation with Empirical Observability Gramian

In this part, we utilize the empirical observability gramians of different sensor configurations for parameter estimation purposes. We model the (empirically determined) fouling parameters α^1 and α^2 as constants up to an additive disturbance effecting their initial conditions, i.e.

$$\dot{\alpha}^j = 0, \; \alpha^j(0) = 0.0005 + w^j, j = 1,2.$$

The Gaussian disturbance terms $w^j \sim \mathcal{N}(0, \Sigma_w)$ are independent and standard deviations are equal to $2.5 * 10^{-5}$, while the initial conditions for the membrane resistances are set similar to the previous case. The perturbation directions and magnitudes are taken as;

$$T^{2,4} = \{I_4, \; -I_4\},$$
$$M = \{\, 2.5, \; 2, \; 1.5, \; 1, \; 0.5\},$$

where we scaled the perturbations with 10^{-5} for the cases perturbing the fouling parameters α^i. The results are tabulated in Figure 3 for four different degree of observability measures. The resulting degree of observability measures are similar with the results of Section 3.2. The cases 5, 6 and 7 are providing the best sensor channels, again, while for the case 3, the information required for estimating the second membrane fouling coefficient is not present in the measurements. Furthermore the output configuration cases 1, 2 and 4 are prone to be numerically problematic for estimation purposes which can be observed by the ill-conditioning of the observability gramian, see the condition number subfigure of Figure 3.

Lastly, to check the validity of the implementation and the results, we designed Kalman filters for the membrane system with the output measurements varying over the measurement channel cases. In Figure 4, we visualize the results for the states and the parameters, including the true values of the states (R_1 and R_2) and the parameters (α^1 and α^2) and the estimation results for the output channel cases 5, 6 and 7. From these results we observe that the optimal output channels are providing an acceptable estimation performance for both of the states and the parameters. The estimation errors of parameters α^i are relatively high but convergent to the true value, however the state trajectories are estimated with high precision for the optimal sensor configurations. For the other sensor configuration cases, which are not reported here, the results are not satisfactory, either due to poor estimation quality of α^i or the true variables being not observable at all.

As an outlook, different degree of observability measures are indicating different aspects of the model. The eigenvalue measure should be used in all cases, to check whether the system is observable or not, however the trace measure is the most reliable one about the informativity of the sensor configuration. The condition number measure indicates whether the estimation algorithm is prone to be numerically erroneous with fastly varying estimates. Since the empirical gramian is calculated through noisy simulation data, it is not advised to make use of determinant measure.

4. CONCLUSION AND FUTURE DIRECTIONS

We consider the optimal sensor configuration problem for an industrial membrane system, represented with unstable nonlinear DAEs, to extract useful information for state and parameter estimation purposes. Several existing methods using the observability gramian's spectral properties to assess the performance of different sensor configurations are discussed. However these gramians are not easily available for unstable nonlinear processes. For this purpose we extend the definition of the empirical observability gramians for unstable nonlinear systems to decide on the optimal sensor configuration. The results show that sensor configuration can be decided based on the empirical observability gramian for estimation purposes. Hence

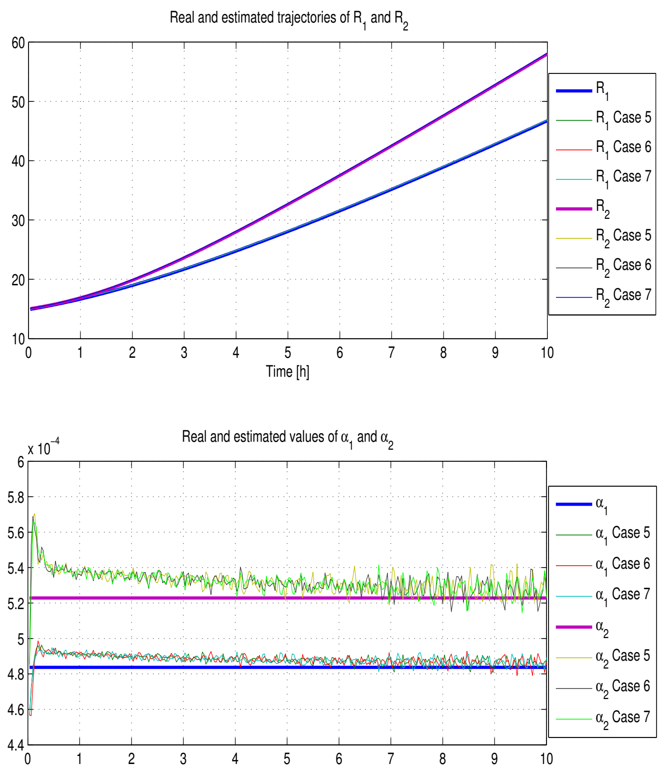

Fig. 4. Simulation results for membrane system. The upper figure visualizes the true and estimated membrane resistance (state) trajectories while bottom figure visualizes the true and estimated fouling coefficient (parameter) trajectories for output channel cases 5, 6 and 7.

the empirical observability gramian, which offers substantial computational benefits, can be used instead of conventional techniques to decide what to measure even if the considered system is unstable and medium to large sized.

Since extensive amount of simulations-perturbations are required to capture the true behaviour of the nonlinear process, we plan to address possible computational complexity reduction schemes for overall online parameter estimation algorithms to calculate the empirical observability gramian.

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