Determining optimal sensor locations for parameter estimation via covariance matrices

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1. Introduction

Online estimation of parameters is significant for control and monitoring of many chemical engineering processes. Accurate estimation of process parameters requires measurements, that ensure observability and a good response of parameter estimates. Therefore, it is highly desirable to place the sensors optimally for estimating process parameters. The problem of sensor placement in chemical processes is aggravated by the fact that most of processes are nonlinear in nature and process disturbances may cause large changes in the parameters.

Most of the available optimality criteria for sensor location for parameter estimation are based on scalar measures of the Fisher information matrix that require computation of a parameter-output sensitivity matrix [4, 6, 7]. In another approach, Li et al. [3] employ principal component analysis on a parameter-output sensitivity matrix in order to compute the best set of parameters that can be estimated for a given measurement locations. All of these techniques require computation of parametric-output sensitivity coefficients that are based on local sensitivity analysis. Therefore, the results obtained by these methods may sometimes be only suitable for small changes in the parameters [8].

This paper presents a new approach of sensor placement for parameter estimation for linear as well as nonlinear systems. The parameters to be estimated are viewed as additional state variables and observability analysis is performed on the augmented system without resorting to linearization. This is achieved by making use of observability covariance matrices for the observability analysis, since the covariance matrices form an extension to the gramians of a linear system. Unlike linear gramians or empirical gramians which require asymptotic stability of the operating region around the equilibrium point, it is sufficient for the computation of the covariance matrices if the system is stable over the investigated operating conditions [2]. This property is essential for sensor location via observability analysis for the augmented system, because the augmented states are not asymptotically stable. Additionally, the covariance matrices capture some of the nonlinear behavior of the system over the region of operation and can be easily computed for nonlinear systems of high complexity and significant size. The information from this investigation is combined with observability measures that have been previously proposed in the literature. This approach offers the advantage over other methods in that it is directly applicable to nonlinear systems without resorting to linearization of the model and hence, can capture part of the nonlinear behavior of the system for large perturbations in the process parameters. The proposed method has been applied to a binary distillation column and fixed bed reactor model. The results have been compared to those obtained by linearizing the model. It is shown that the optimal sensor locations determined by the presented procedure are in line with predictions from physical insight into the model. This is in stark contrast to methods relying on linearization which have been applied to these models and return locations which are non-optimal for the nonlinear system under study.

2. Sensor location procedure

In order to compute the optimal sensor location for parameter estimation, the nonlinear system given by (1) is augmented with equations of parameter (p) to be estimated.

$$\dot{x} = f(x,p,u) \tag{1a}$$
$$y = h(x,p,u) \tag{1b}$$

The parameters are assumed to be constant or slow varying and therefore they can be described by $\dot{p} = 0$. The parameter equations are added to system described by (1) and the augmented nonlinear system is given by:

$$\begin{pmatrix} \dot{x} \\ \dot{p} \end{pmatrix} = \begin{pmatrix} f(x,p,u) \\ 0 \end{pmatrix} \tag{2a}$$
$$y = h(x,p,u) \tag{2b}$$

To compute optimal measurements, observability analysis is performed on the augmented system described by (2). If the system is linearized, then it will have as many zero eigenvalues as there are unknown parameters. Hence, linear gramians $(W_{O,linear})$ cannot be used for the observability analysis of the linearized system as $W_{O,linear} \to \infty$ for marginally stable system. Similarly, linear gramians cannot be used for observability analysis if the system is linear. However, observability covariance matrices do not have this restriction.

The observability covariance matrix [3] is defined as:

$$W_O = \sum_{l=1}^{r} \sum_{m=1}^{s} \frac{1}{(rsc_m^2)} \int_0^{\infty} T_l \Psi^{lm}(t) T_l^T dt \tag{3}$$

where $\Psi^{lm}(t) \in R^{n\times n}$ corresponds to $\Psi_{ij}^{lm}(t) = (y^{ilm}(t) - y_{ss})^T (y^{jlm}(t) - y_{ss}), y^{ilm}(t)$ is the output of the system corresponding to the initial condition $x(0) = c_m T_l e_i + x_{ss}$, and y_{ss} is the steady state output of the system. The matrix T in the above definition is given by:

$$T^n = \{T_1, ..., T_r; T_i \in R^{n\times n}, T_i^T T_i = I, i = 1, ..., r\}$$

and r, s, n represent the number of matrices for the perturbation directions, the number of different perturbation sizes for each direction, and the number of states of the system respectively.

These covariance matrices can be used for the observability analysis of augmented linear or linearized system and they reduce to the linear observability gramian if the linear system is asymptotically stable. The observability covariance matrix captures the nonlinear behavior of the system over the operating region and hence it can be used for observability analysis of the nonlinear system.

The computed observability covariance matrix of the augmented system can be decomposed as follows:

$$W_O = \begin{pmatrix} W_{O,nn} & W_{O,np} \\ W_{O,pn} & W_{O,pp} \end{pmatrix} \tag{4}$$

where the submatrix $W_{O,nn}$ represents the observability covariance matrix of the system (2) before augmentation with the parameters as additional states, $W_{O,pp}$ represents the variance-covariance of the parameters, and $W_{O,np}$ and $W_{O,pn}$ represent the covariances of the state variables and parameters. If the rank of the augmented observability covariance matrix (4) is equal to the sum of the number of states and parameters then the augmented system is observable and the parameters can be estimated. The degree of observability of the set of parameters is determined by the submatrix $W_{O,pp}$ since it represents the covariance matrix of the parameters. The diagonal elements of this matrix represent the variance that changes in the parameters cause in the outputs and the other entries are an indicator for the degree of interaction between the parameters. Hence, measures based on the sub-matrix $W_{O,pp}$ can be used to determine the best sensor location for parameter estimation.

$$\omega = measure(W_{O,pp}) \tag{5}$$

Measures like trace and norm of the observability covariance matrix can be used to estimate the degree of observability of the parameters. For the case where only a single process parameter needs to be estimated, the $W_{O,pp}$ matrix reduces to a scalar which needs to be maximized.

3. Results

The new method for sensor location has been applied to two examples. In the first example a model of binary distillation column [1] is considered and the optimal location for estimating the relative volatility is computed. In the second example an infinite-dimensional model of a fixed bed reactor [5] is investigated.

Distillation Column

In order to compute optimal locations for estimating relative volatility in column, the observability covariance matrix is computed for all possible measurements, i.e. measuring each of the 32 states individually. Observability analysis is performed for each of the computed covariance matrices. The submatrix $W_{O,pp}$ is extracted from the observability matrix. As only one parameter is determined $W_{O,pp}$ reduces to a scalar that is maximized over the entire set of possible measurement to obtain the best sensor location.

While analyzing the results obtained for sensor location for the column (Figure 1), it can be seen that the best location for parameter estimation is 8th tray. In order to corroborate these findings, the performance of a Kalman filter is compared for the optimal and a non-optimal measurement. The results indicate faster convergence of the Kalman filter for parameter estimation when the measurements are placed at the optimum location.

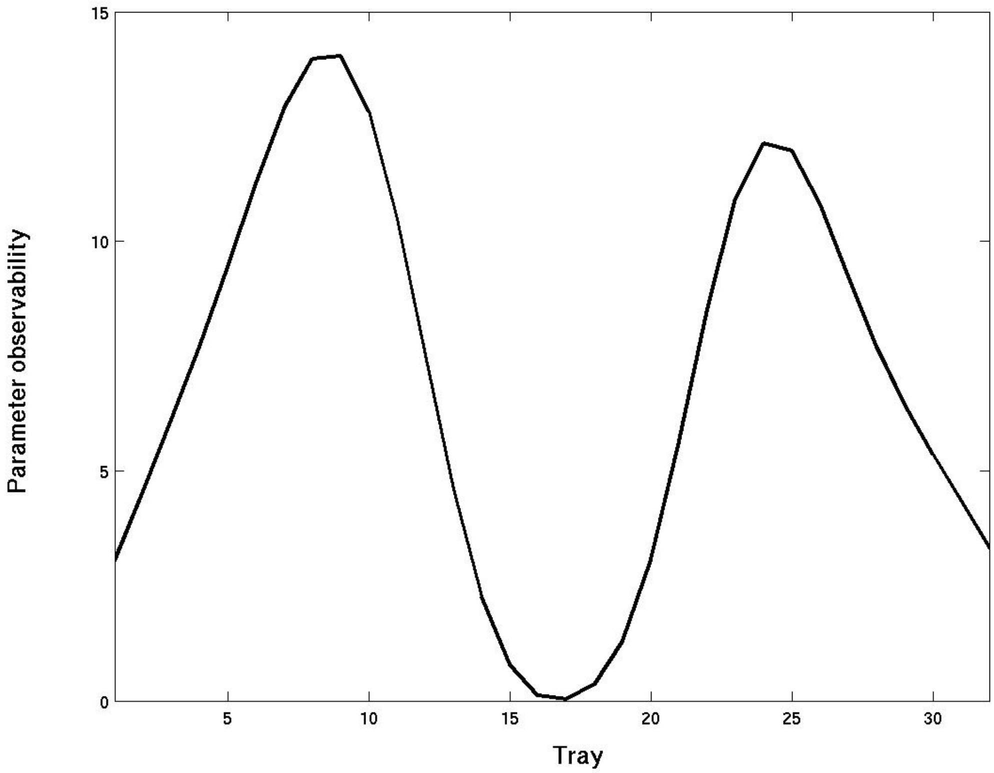

Figure 1. Values of the measure for placing a sensor on the distillation column for estimating relative volatility.

Fixed-bed reactor

In this example, the optimal location for estimating the feed inlet temperature is computed. Similar analyses can be carried out for locating the best measurement in a reactor for estimating other parameters like the heat transfer coefficient or the activation energy. The optimal measurement location is computed for the nonlinear reactor model as well for a linearized version of nonlinear model for 5% uncertainty in the parameter. The optimal location obtained from the nonlinear model is at 0.2 m from the rector inlet while for the linearized model it is almost at the inlet of the reactor (Figure 2). If the nonlinear reactor model is simulated for 5% uncertainty in the process parameter, it can be observed that in fact the location provided by nonlinear model is physically meaningful as the sensor location by nonlinear model is within the ranges of hotspot locations for 5% change in the process parameter. The results returned for the linear model, on the other hand, do not correspond to a physically meaningful location.

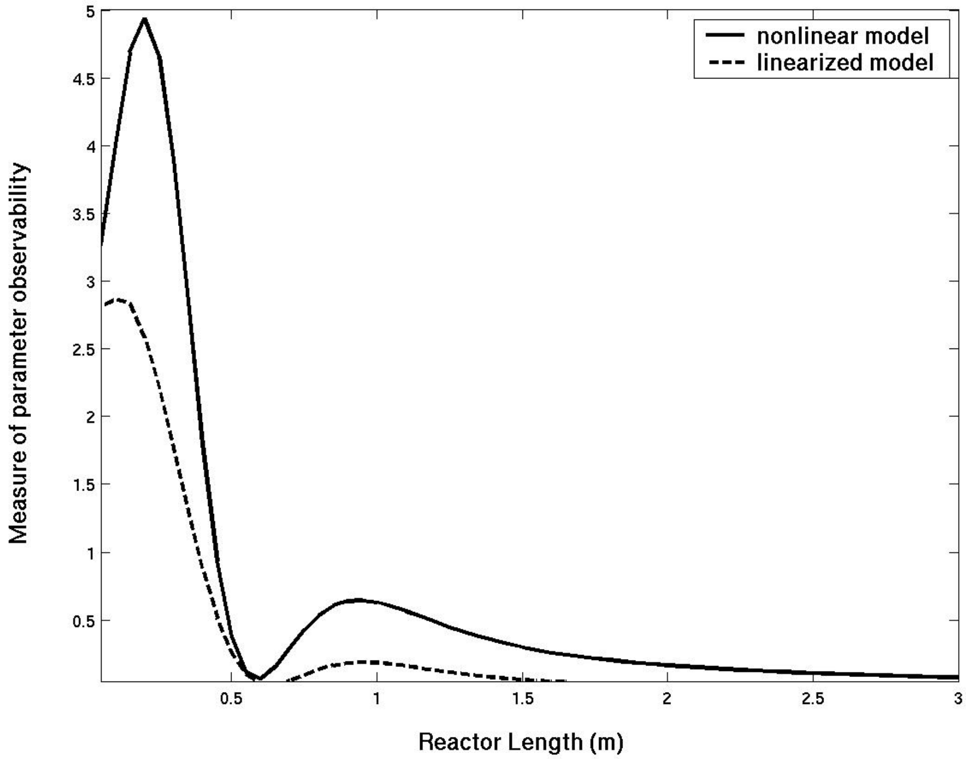

Figure 2. Values of the measure for placing a temperature sensor along the length of the reactor for parameter estimation.

4. Conclusions

This paper presents a new technique for estimating sensor locations for parameter estimation for linear as well as nonlinear systems. This method has the advantage that it can be applied to nonlinear systems without resorting to linearization and the results are valid for large perturbations in the process parameters.

This methodology has been applied to two examples, i.e. a distillation column and a fixed bed reactor. The computed locations are in line with predictions from physical insight into the models. Additionally, parameter estimation via a Kalman filter has been performed and it was determined that the estimation works better if the measurement is placed at the computed optimal location.

References

[1] Benallou, A.; Seborg, D.E.; Mellichamp, D.A. Dynamic compartmental models for separation processes. *AIChE Journal* **1986,** 32, 1067.
[2] Hahn, J.; Edgar,T.F.; Marquardt, W. Controllability and observability covariance matrices for the analysis and order reduction of stable nonlinear systems. *Journal of Process Control* **2003**, 13, 115.
[3] Li, R.; Henson, M.A.; Kurtz, M.J. Selection of model parameters for off-line parameter estimation. *IEEE Transaction on Control System Technology* **2004**, 12, 402.
[4] Quershi, Z.H.; Ng, T.S.; Goodwin, G.C. Optimum experimental design for identification of distributed systems. *International Journal of Control* **1980**, 31, 21.
[5] Van Welsenaere, R.J. Van; Froment, G.F. Parameter sensitivity and runaway in fixed bed catalytic reactors. *Chemical Engineering Science* **1970**, 25, 1503.
[6] Walter, E.; Pronzato, L. Qualitative and quantitative experiment design for phenomenological models-a survey. *Automatica* **1990**, 26, 195.
[7] Wouwer, A.V.; Point, N.; Porteman, S.; Remy, M. An approach to the selection of optimal sensor locations in distributed parameter systems, *Journal of Process Control* ***2000***, 10, 291.
[8] Varma, A.; Morbidelli, M.; Wu, H. *Parametric Sensitivity in Chemical Systems*; Cambridge University Press: Cambridge, U.K.,1999