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PROCESS DESIGN AND CONTROL

A Gramian Based Approach to Nonlinearity Quantification and Model Classification

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This paper introduces a new method for quantifying the nonlinearity of a process. The approach compares the controllability and observability gramians of a system that is linearized at its steady state operating point to empirical gramians, which are computed from data collected within an operating region of the nonlinear process. This comparison results in two measures for the nonlinearity of the input−output behavior of a process: one for the nonlinearity in the input-to-state behavior (controllability) and one for the nonlinearity in the state-to-output behavior (observability). This is important for controller/observer design, as well as model reduction, because it indicates when it is appropriate to replace a nonlinear model with a linearization around its operating point. In addition, severely nonlinear models can be identified as being Wiener-like models, Hammerstein-like models, or nonlinear in both input-to-state and state-to-output behavior. The proposed approach is illustrated with several examples comparing this method with nonlinearity measures used in the literature.

1. Introduction

Most dynamic systems in chemical engineering exhibit some kind of process nonlinearity which can range from mild to severe. When such a process is modeled by nonlinear differential equations, normally the nonlinear model is harder to use in on-line control-related calculations than a model derived from a linearization around an operating point. In some cases the nonlinear model cannot be solved on-line due to the required computation times. On the other hand, linearized models give a good description of the system behavior close to an operating point, but can perform poorly when the process is operated in a larger region. The size of the region where the linear approximation is valid depends on the nonlinearity of the process.[1]

This paper introduces a method of measuring the nonlinearity of a control-affine process over a given operating region. This measurement of open loop nonlinearity is in contrast to methods that measure the nonlinearity of a control law, but the method presented here can provide quantification of the nonlinearity before a controller is designed, as is the case for closed loop nonlinearity assessment. The proposed measures analyze the nonlinearity of the process in the input-to-state as well as the state-to-output behavior. The measures indicate if it is appropriate to work with the linearization of the model within this operating region or if substantial benefits can be gained by using the nonlinear model. Additionally, if a model contains severe nonlinearities, it can be classified as being Wiener-like, Hammerstein-like, or nonlinear in both input-to-state and state-to-output behavior.

The nonlinearity measures are computed by comparing the observability and controllability gramians of the linear model to empirical observability and controllability gramians of the nonlinear systems after a balancing transformation on both systems has been performed. One advantage of this method is that it determines how relevant the nonlinearities are to the control of the system. If a system includes highly nonlinear states, which are only barely observable or controllable, they will have little effect on the nonlinearity of the input−output behavior of the system. A further advantage is that the procedure is computationally inexpensive.

Another byproduct of this nonlinearity assessment is that the results can directly be used for nonlinear model reduction. If it is determined that a linear model for a given process under specified operating conditions does not reflect the dynamic behavior appropriately and at the same time the nonlinear model is too computationally intensive for on-line application, then nonlinear model reduction techniques are required. The empirical gramians from which the nonlinearity measures are computed can then be used within a model reduction scheme as shown by Hahn and Edgar.[2,3]

2. Previous Work: Nonlinearity Measure

Most nonlinearity measures are concerned with the open loop nonlinearity of a system by comparing the behavior of a linear model with the original nonlinear model. Several different approaches for finding a linear model and comparing its input−output behavior to that of the nonlinear system have been proposed. Nonlinearity measures were first used by Desoer and Wang[4] to quantify the degree of the nonlinearity of the input−output mapping of a system. Their technique used an approximated linearized system for the computation of

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the measure. Haber[5] proposed several methods that can verify if the input−output mapping is linear, but not their degree of nonlinearity. Nikolaou[6] and Nikolaou and Hanagandi[7] used Monte Carlo simulations together with an inner product in order to evaluate differences between the best linear model for different inputs and the nonlinear system. Allgöwer[8] used simulations to determine the difference between the best linear model for the worst input signal and its nonlinear counterpart near a stable steady state operating point. This method was extended by Helbig et al.[9] in order to be applicable at points that are unstable or even along predetermined trajectories. Guay et al.[10] quantified steady state nonlinearities by using curvature metrics of the steady state locus. The same authors later extended their method to dynamic nonlinearities by using an operator framework.[11] Sun and Hoo[12] measured system nonlinearity of SISO systems by computing the upper and lower linear boundaries of the nonlinear system. They stated that a controller that provides satisfactory performance for the two bounding linear systems will result in good performance for the nonlinear system as well. Harris et al.[13] proposed an approach to compute the nonlinearity measure by Allgöwer[8] using functional expansions. The described method derives upper and lower bounds for the degree of nonlinearity and is computationally inexpensive.

Instead of focusing on open loop systems, Stack and Doyle[14,15] investigated the nonlinearity of an optimal controller for a nonlinear system. Their approach is based upon the fact that although some systems are nonlinear in nature they show good performance when controlled by a linear controller. Coherence analysis,[16] which is a statistical technique, was used in order to determine nonlinearity of the required optimal control law.

3. Gramian Based Nonlinearity Measures

The method proposed in this paper quantifies nonlinearity by comparing input−output behavior of the nonlinear system to the behavior of the system that results from linearizing at the steady state operating point. The nonlinearity measure involves computation of the observability and controllability gramians for the linear system and computation of the empirical gramians for the nonlinear model. The next section presents the computation procedure for empirical gramians. Section 3.2 will present how discrete empirical gramians are computed and gives more details on the algorithm used in order to determine a balancing transformation. The nonlinearity measures for both controllability and observability are introduced in section 3.3.

3.1. Empirical Gramians. Empirical gramians are defined for stable and control-affine nonlinear systems as given by eq 1.

$$\begin{aligned}\dot{x}(t) &= f(x(t)) + g(x(t))\,u(t)\\ y(t) &= h(x(t))\end{aligned} \tag{1}$$

The following sets need to be defined for empirical gramians:

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

$$M = \{c_1, ..., c_s;\ c_i \in \mathscr{R},\ c_i > 0,\ i = 1, ..., s\}$$

$$E^n = \{e_1, ..., e_n;\ \text{standard unit vectors in } \mathscr{R}^n\}$$

where

r is the number of matrices for perturbation directions

s is the number of different perturbation excitation sizes for each direction

n is the number of inputs to the system for the controllability gramian and number of states of the full-order system for the observability gramian

The following quantities are defined:

Empirical Controllability Gramian. *Let T^p, E^p, and M be given sets as described above, where p is the number of inputs. The empirical controllability gramian is defined by*

$$W_{\mathrm{C}} = \sum_{l=1}^{r}\sum_{m=1}^{s}\sum_{i=1}^{p}\frac{1}{rsc_m^{\,2}}\int_0^{\infty}\Phi^{ilm}(t)\,\mathrm{d}t \tag{2}$$

where $\Phi^{ilm}(t) \in \mathscr{R}$ is given by $\Phi^{ilm}(t) = (x^{ilm}(t) - x_{ss}{}^{ilm})(x^{ilm}(t) - x_{ss}{}^{ilm})^{\mathrm{T}}$, and $x^{ilm}(t)$ is the state of the nonlinear system corresponding to the impulse input $u(t) = c_m T_l e_i \delta(t) + u_{ss}$.

Empirical Observability Gramian. *Let T^n, E^n, and M be given sets as described above, where n is the number of states. The empirical observability gramian is defined by*

$$W_{\mathrm{O}} = \sum_{l=1}^{r}\sum_{m=1}^{s}\frac{1}{rsc_m^{\,2}}\int_0^{\infty}T_l\Psi^{lm}(t)T_l^{\mathrm{T}}\,\mathrm{d}t \tag{3}$$

where $\Psi^{lm}(t) \in \mathscr{R}^{n\times n}$ is given by $\Psi^{lmij}(t) = (y^{ilm}(t) - y_{ss}{}^{ilm})^{\mathrm{T}}(y^{jlm}(t) - y_{ss}{}^{jlm})$, and $y^{ilm}(t)$ is the output of the nonlinear system corresponding to the initial condition $x(0) = c_m T_l e_i + x_{ss}$.

Lall et al.[17,18] have shown that both of these empirical gramians reduce to linear gramians for linear models. Furthermore, the empirical gramians will reduce to gramians of the linearized system for small perturbations around the operating point.

These empirical gramians are determined from simulation data, collected within a region where the process is to be controlled. The empirical gramian matrices capture part of the nonlinear behavior within the region of operation and therefore can be used for nonlinearity quantification when they are compared to gramians of a linear system.

The empirical gramians are only defined for control-affine models due to the fact that an impulse input will lead to different behavior for non-control-affine models, depending upon the implementation of the impulse as a pulse of finite time and magnitude. While it is possible to draw some conclusions about the qualitative behavior if empirical gramians are computed for a non-control-affine system, these results should not be used for quantitative analysis or even model reduction.

3.2. Computational Procedure. Since empirical gramians are by their nature based upon discrete measurements of system properties, like states and outputs, it is advantageous to reformulate them in a discrete form. Therefore the following quantities are defined:

Discrete Empirical Controllability Gramian. *Let T^p, E^p,* and *M be given sets as described in section 3.1, where p is the number of inputs. The discrete empirical controllability gramian is defined by*

$$W_C = \sum_{l=1}^{r} \sum_{m=1}^{s} \sum_{i=1}^{p} \frac{1}{rsc_m^2} \sum_{k=0}^{q} \Phi_k^{ilm} \Delta t_k \tag{4}$$

where $\Phi_k^{ilm} \in \mathcal{R}$ *is given by* $\Phi_k^{ilm} = (x_k^{ilm} - x_{ss}^{ilm})(x_k^{ilm} - x_{ss}^{ilm})^T$, *and* x_k^{ilm} *is the state of the nonlinear system corresponding to the impulse input* $u_k = c_m T_l e_i \delta_{k=0} + u_{ss}$.

The controllability gramian can be viewed as the sum of the variance−covariance matrix of the states over time and for different combinations of the input variables. These combinations include different input directions (given by the choice of $T_l e_i$) as well as magnitudes (fixed by the choice of c_m) and should include all relevant cases for a specific model according to the design instructions for these inputs given by the choice of T^n.

Discrete Empirical Observability Gramian. *Let* T^n, E^n, *and M be given sets as described in section 3.1, where n is the number of states. The discrete empirical observability gramian is defined by*

$$W_O = \sum_{l=1}^{r} \sum_{m=1}^{s} \frac{1}{rsc_m^2} \sum_{k=0}^{q} T_l \Psi_k^{lm} T_l^T \Delta t_k \tag{5}$$

where $\Psi_k^{lm} \in \mathcal{R}^{n\times n}$ *is given by* $\Psi_k^{lm}{}_{ij} = (y_k^{ilm} - y_{ss}^{ilm})^T(y_k^{jlm} - y_{ss}^{jlm})$, *and* y_k^{ilm} *is the output of the* nonlinear *system at time step k corresponding to the initial condition* $x_0 = c_m T_l e_i + x_{ss}$.

The observability gramian can be interpreted as the sum of the variance−covariance matrix of the outputs, corresponding to different initial conditions, and over time.

Although these gramians are computed from discrete data points, the data reflects the states and output measurements of a continuous system given by eq 1 at a specified time. The variables q and Δt_k need to be chosen in such a way that the system will have reached steady state at some $k < q$ for any kind of impulse input (controllability) or state perturbation (observability). For the purpose of this paper the value of q was set to greater than 2000 for the examples shown in section 4 in order to ensure that the system behavior is correctly reflected in the data. The size of the time steps was fixed for each problem and the value determined from the longest settling time computed for the excitations/perturbations in accordance with the computation procedure for the empirical gramians.

To formulate the nonlinearity measures, a balancing transformation needs to be applied to the gramians. The proof that for two symmetric positive semidefinite matrices, such as the gramians, there always exists a transformation that balances the system can be found in Zhou and Doyle.[19] An algorithm that balances systems when both of these matrices are symmetric positive definite and thereby the system is completely observable and controllable can be found in the same reference. The description of an algorithm that computes a balancing transformation for the empirical gramians of any system is given below.

1. In a first step the uncontrollable modes are identified and removed. This is done via a Schur decomposition of the controllability gramian as shown in eq 6. If the diagonal matrix $W_{C,\text{diagonal}}$ does not contains its largest element in the first row and column, then the transformation has to be multiplied by a permutation matrix that reorders the states of the system. The rank of the controllability gramian W_C is equal to the number of controllable states n_C in the system.

$$W_C = T_C W_{C,\text{diagonal}} T_C^T \tag{6}$$

$$n_C = \text{rank}(W_C) \tag{7}$$

$$\tilde{T}_C = [T_C(1{:}n,1{:}n_C)\ \ \text{zeros}(n,n - n_C)] \tag{8}$$

2. In a next step these uncontrollable states are removed from the observability gramian as is shown in eqs 9 and 10. Following this the unobservable but controllable states are identified via another Schur decomposition as shown in eq 11. If the diagonal matrix $W_{O,\text{diagonal}}$ does not contains its largest element in the first row and column, then the transformation has to be multiplied by a permutation matrix that reorders the states of the system.

$$\tilde{W}_O = \tilde{T}_C^T W_O \tilde{T}_C \tag{9}$$

$$\hat{W}_O = \tilde{W}_O(1{:}n_C,1{:}n_C) \tag{10}$$

$$\hat{W}_O = T_O W_{O,\text{diagonal}} T_O^T \tag{11}$$

$$n_{CO} = \text{rank}(W_{O,\text{diagonal}}) \tag{12}$$

$$\tilde{T}_O = \begin{bmatrix} T_O(1{:}n_{CO},:) & \text{zeros}(n_{CO},n - n_{CO}) \\ \text{zeros}(n - n_{CO},n_{CO}) & \text{zeros}(n - n_{CO},n - n_{CO}) \end{bmatrix} \tag{13}$$

$$T_{CO} = \tilde{T}_C \tilde{T}_O \tag{14}$$

3. The gramians for the subsystem that is both controllable and observable are given by eqs 15 and 16, and the rank of this system is n_{CO}. Since only the first n_{CO} rows and columns of these gramians are nonzero, the rows and columns containing zeros can be truncated. Since the remaining subsystem is both controllable and observable, the general balancing algorithm as described by Zhou and Doyle[19] can be applied to it, resulting in an invertible balancing transformation T.

$$\bar{W}_C = T_{CO}^T W_C T_{CO} \tag{15}$$

$$\bar{W}_O = T_{CO}^T W_O T_{CO} \tag{16}$$

Eliminating the parts of the system that are either uncontrollable or unobservable will not change the input−output behavior of the system and therefore will have no effect on the degree of nonlinearity of the input−output behavior.

3.3. Nonlinearity Measures. The nonlinearity in the input−output behavior of a process can be described by nonlinearities in the input-to-state and in the state-to-output behavior for state space models. Nonlinearity in the input-to-state behavior is described by differences in the dynamics of states between the nonlinear and linear model caused by the input. This will be called input nonlinearity. State-to-output nonlinearity on the other hand will be called output nonlinearity, and it describes deviations in the dynamics of the outputs of the nonlinear model from the linear system caused by perturbations in the states. The nonlinearity of the input−output behavior of the system is given by both measures.

The computation of the two nonlinearity measures requires two gramians for each measure. One is the controllability/observability gramian of the linear system, and the other is the corresponding empirical gramian. Since the empirical gramians reduce to linear gramians for very small perturbations,[17,18] the nonlinearity for a small operating region is always zero. This can be seen in the examples in section 4 as well. After the computation of all four gramians, the transformation that balances the gramians of the linear system is computed by the procedure shown in section 3.2. After the balancing transformation the linear gramians are identical and equal to a diagonal matrix as shown in eq 17 which can be interpreted as each state of the system being just as important for the input-to-state behavior as for the state-to-output behavior.[19] Comparing gramians of the balanced system has the advantage that it can determine if the input−output behavior of the nonlinear system deviates from its behavior for the linearized model. If a state is highly nonlinear in its input-to-state behavior, but does not affect the state-to-output behavior at all, then it will not influence the input−output behavior. This will be clear for a balanced system, but may not be the case if the system is not balanced.

The balancing transformation is determined by the procedure in section 3.2 and a general balancing algorithm,[19] and then applied to the empirical gramians of the nonlinear system as well as shown in eqs 18 and 19.

$$\bar{W}_{L} = T_{CO}{}^{T} T^{-1} W_{C,LINEAR} (T^{-1})^{T} T_{CO} = T_{CO}{}^{T} T^{T} W_{O,LINEAR} T T_{CO} \qquad (17)$$

$$\bar{W}_{C,N} = T_{CO}{}^{T} T^{-1} W_{C,NONLINEAR} (T^{-1})^{T} T_{CO} \qquad (18)$$

$$\bar{W}_{O,N} = T_{CO}{}^{T} T^{T} W_{O,NONLINEAR} T T_{CO} \qquad (19)$$

Now the two nonlinearity measures can be defined:

Input Nonlinearity Measure. *The input nonlinearity measure is defined by*

$$\Phi_{C} = \frac{\sum_{i=1}^{n}\sum_{j=1}^{n} |\bar{W}_{L}(i,j) - \bar{W}_{C,N}(i,j)|}{\sum_{i=1}^{n} \bar{W}_{L}(i,i)} \qquad (20)$$

where the first entry of the ordered pair of matrices indicates the row and the second entry the column. Each ordered pair refers to a specific element of the matrix.

Output Nonlinearity Measure. *The output nonlinearity measure is defined by*

$$\Phi_{O} = \frac{\sum_{i=1}^{n}\sum_{j=1}^{n} |\bar{W}_{L}(i,j) - \bar{W}_{O,N}(i,j)|}{\sum_{i=1}^{n} \bar{W}_{L}(i,i)} \qquad (21)$$

where the first entry of the ordered pair of matrices indicates the row and the second entry the column.

The input nonlinearity measure is determined by the weighted sum of the absolute values of the difference of each element of the covariance matrices due to changes in the inputs. The output nonlinearity measure is defined similarly. Both measures will be zero for linear systems since empirical gramians reduce to ordinary gramians for linear systems as well as for small excitations/perturbations around the operating point. However, for large excitations/perturbations and strongly nonlinear models the measures will approach high values, due to the fact that the states of the nonlinear model will have covariances different from zero for a nonlinear model that is simulated in a large operating region. Both measures can at least theoretically approach infinity for extreme nonlinearities, but a value of unity will already indicate a strongly nonlinear system. This is due to the fact that the difference in the covariance caused by the nonlinearities in the process will be just as large as the variances of the process states for a nonlinearity measure of unity.

This method can be applied to SISO as well as to MIMO systems, due to the fact that no assumptions were made in this regard. The computation procedure of the empirical gramians can be applied to MIMO systems without any modification. The same is true of the computation of the transformation matrix and the nonlinearity measures.

3.4. Model Classification. Based upon the two nonlinearity measures models can be classified as belonging to one of the following four categories for a prespecified operating region.

1. Linear or mildly nonlinear models: These models will have low input and output nonlinearity measures over the whole operating region.

2. Wiener-like models: A Wiener-like model will have a low input nonlinearity measure, but a high output nonlinearity measure for at least some values in the operating region. A real Wiener process as given by eq 22 will have an input nonlinearity of zero for the whole operating region, but does exhibit output nonlinearity.

$$\begin{aligned} \dot{x}(t) &= Ax(t) + Bu(t) \\ y(t) &= h(x(t)) \end{aligned} \qquad (22)$$

Simulations have shown that the nonlinearity measures will correctly identify this behavior and the input nonlinearity measure is indeed exactly zero for a real Wiener process.

3. Hammerstein-like models: These models will have a low output nonlinearity measure and an input nonlinearity behavior that cannot be classified as linear. A real Hammerstein process as given by eq 23 will have no output nonlinearity, but will exhibit input nonlinearity.

$$\begin{aligned} \dot{x}(t) &= Ax(t) + g(u(t)) \\ y(t) &= Cx(t) \end{aligned} \qquad (23)$$

This result from Stack and Doyle[15] can be reproduced with the given measure; even so a real Hammerstein process is not control-affine.

4. Nonlinear models in both input-to-state and state-to-output behavior.

Mildly nonlinear systems can usually be treated as linear for controller/observer design purposes as well as for model reduction. Models nonlinear in their input and output behavior must be treated as such, whereas specialized controller/observer design procedures can be used for Wiener or Hammerstein models.

4. Application of the Measures to Examples

The nonlinearity measure described in section 3 has been applied to several examples used by other research-

Table 1. Parameters for the CSTR Given by System (24)−(26)

variable	value
$x_{1,ss}$	0.143 969 2
$x_{2,ss}$	0.885 964 8
u_{ss}	1.0
γ	20.0
β	0.3
B	8.0
Da	0.072

ers. In the following examples the results from the Gramian−based nonlinearity measures are compared with other methods.[7,13,14] The presented examples exhibit varying degrees of nonlinearity.

Example 1: Mildly Nonlinear CSTR. Nikolaou and Hanagandi[7] investigated the nonlinearity behavior of a CSTR given by eqs 24−26. The parameters for this problem can be found in Table 1.

$$\frac{dx_1}{dt} = -x_1 + Da(1 - x_1)\exp\left(\frac{x_2}{1 + \frac{x_2}{\gamma}}\right) \quad (24)$$

$$\frac{dx_2}{dt} = -x_2 + BDa(1 - x_1)\exp\left(\frac{x_2}{1 + \frac{x_2}{\gamma}}\right) + \beta((u - 1) - x_2) \quad (25)$$

$$y = x_2 \quad (26)$$

This system describes a constant-volume CSTR with one reaction. The state variable x_1 refers to the dimensionless concentration of the reactant species in the reactor, and the second state variable x_2 represents the dimensionless reactor temperature. The system is a SISO system where the only control is the normalized cooling jacket temperature u and the reactor temperature x_2 is the measurement.

Nikolaou and Hanagandi[7] concluded by means of their method that this reactor exhibits only mild nonlinearities in the input−output behavior.

The empirical gramians of this system were computed by simulating the system under various conditions, consistent with the description given in section 3.2. The time step size Δt was chosen to be 0.01 and q equal to 2000 for this example to ensure that a sufficient number of data points were used for the computation of the empirical gramians. The simulations were plotted to verify that the system reaches its original steady state within the simulated time for each of the chosen operating conditions. Next, the values of the empirical gramians for small excitations/perturbations around the operating point were compared to the gramians of the linearized system that were computed using standard MATLAB routines. Both were found to be virtually identical for small perturbations resulting in a nonlinearity measure close to zero. Consequently, the size of the excitations/perturbations was increased up to a value of 90% around the steady state and the nonlinearity of the system increased accordingly as is shown in Figure 1. The states as well as the inputs to the system were scaled to evaluate the effect that the excitations/perturbations have on the system. The variable c_m in Figure 1 refers to the size of the excitations/perturbations used for the computation of the empirical gramians eqs 4 and 5. It should be noted that since the

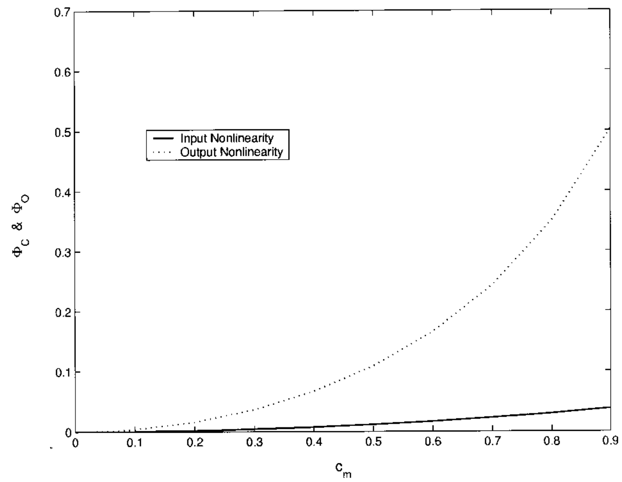

Figure 1. Input and output nonlinearity measures for example 1.

input nonlinearity is computed from the empirical controllability gramian, it must be based upon impulse inputs to the system. In this case a 10% excitation means that the system is subjected to a pulse where the pulse height multiplied by the pulse width equals 0.1. This is distinctly different from applying step changes of 10% of the input to the system, in that the step change is likely going to drive the system further away from the operating point and will result in more severe nonlinear behavior.

For these operating conditions the system exhibits only small nonlinearity in the input-to-state behavior over the whole range. The state-to-output behavior is more nonlinear but the nonlinearity measure remains low (less than 0.1) up to perturbations of 50% around the steady state values. Since both measures are relatively small over a large range the system exhibits only mildly nonlinear behavior for these operating conditions. These observations are comparable with the results of Nikolaou and Hanagandi[7]. This model can be either classified as a mildly nonlinear system or a Wiener process depending upon the operating region under investigation.

Example 2: Isothermal CSTR with van de Vusse Reaction. Harris et al.[13] applied their nonlinearity measure to an isothermal, perfectly mixed, nonlinear CSTR governed by the van de Vusse reaction kinetics shown in eq 27.

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$
$$A \xrightarrow{k_3} D \quad (27)$$

The first and second reactions in the van de Vusse reaction scheme have first-order kinetics, whereas the third reaction is of second order. This system can be described by the two nonlinear differential equations given by (28) and (29).

$$\frac{dC_A}{dt} = -k_1C_A - k_3{C_A}^2 + \frac{u}{V}(C_{A,Feed} - C_A) \quad (28)$$

$$\frac{dC_B}{dt} = k_1C_A - k_2C_B - \frac{u}{V}C_B \quad (29)$$

$$y = C_B \quad (30)$$

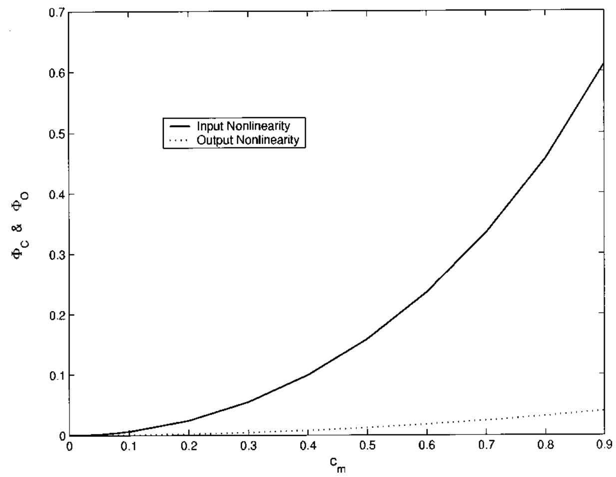

Figure 2. Input and output nonlinearity measures for example 2.

The inlet flow rate u is the manipulated variable of the system, while the output is given by the concentration C_B, making this a SISO system. The parameters for the system are summarized in Table 2.

Harris et al.[13] found that this system exhibits mildly nonlinear behavior in the operating region under investigation. This region was given by constraining the input to be in the interval [19.3 L/h, 49.3 L/h], which is approximately equal to a 50% step change of the input around its steady state.

The time steps, Δt, for this problem were chosen to be 0.001 min, and q was set to 5000 to reflect the dynamic behavior of the process within the empirical gramians. The size of the excitations/perturbations was varied from 0 to 90% for the computation of the nonlinearity measures. Unlike in example 1, the input-to-state behavior deviated more from the behavior of the linear system than the state-to-output behavior, as can be seen in Figure 2. This indicates a Hammerstein-like process, assuming the operating region is chosen large enough such that the process exhibits nonmild input nonlinearities.

The state-to-output behavior exhibits very mild nonlinearity over the whole range of excitations of up to 90%. The input-to-state behavior stays fairly linear over a wide range of operating conditions since the input nonlinearity measure has a value of approximately 0.15 for changes in the input of 50%. Therefore, the input–output behavior of the system is only mildly nonlinear in this range, similar to the results by Harris et al.[13]

Example 3: Production of Cyclopentanol in a CSTR. Stack and Doyle[14] investigated a CSTR that describes the production of cyclopentanol from cyclopentadiene, with a number of competing side reactions. The reactions follow a van de Vusse scheme and are given by eq 31.

$$\mathrm{A} \xrightarrow{k_1} \mathrm{B} \xrightarrow{k_2} \mathrm{C}$$

$$2\mathrm{A} \xrightarrow{k_3} \mathrm{D} \tag{31}$$

Component A is the reactant cyclopentadiene, B refers to the product cyclopentanol, and C and D are the unwanted side products cyclopentandiol and dicylopentadiene. The system is described by three differential equations given by (32)–(34). Unlike example 2, this reactor model includes an energy balance and will therefore have the potential to exhibit more severe nonlinear behavior than example 2.

Table 2. Parameters for the CSTR Given by System (28)–(30)

variable	value
$C_{A,ss}$	3.0 mol/L
$C_{B,ss}$	1.12 mol/L
u_{ss}	34.3 L/h
k_1	50 h^{-1}
k_2	100 h^{-1}
k_3	10 h^{-1}/(mol h)
$C_{A,Feed}$	10 mol/L
V	1.0 L

Table 3. Parameters for the CSTR Given by System (32)–(36)

variable	value
k_1	1.287×10^{12} h^{-1}
k_2	1.287×10^{12} h^{-1}
k_3	9.043×10^{9} h^{-1}/(mol h)
E_1/R	9758.3 K
E_2/R	9758.3 K
E_3/R	8560.0 K
ΔH_1	4.2 kJ/mol
ΔH_2	−11.0 kJ/mol
ΔH_3	−41.85 kJ/mol
$C_{A,Feed}$	5.1 mol/L
T_{Feed}	403.15 K
V	10.0 L
Q	−4496 kJ/h
ρ	0.9342 kg/L
c_P	3.01 kJ/(kg K)

Table 4. Parameters for the Two Operating Points

variable	A	B
$C_{A,ss}$	2.4946 mol/L	1.0562 mol/L
$C_{B,ss}$	1.1004 mol/L	0.8123 mol/L
T_{ss}	411.08 K	399.02 K
u_{ss}	800.0 L/h	92.5 L/h

$$\frac{dC_A}{dt} = \frac{u}{V}(C_{A,Feed} - C_A) - k_1 C_A - k_3 {C_A}^2 \tag{32}$$

$$\frac{dC_B}{dt} = -\frac{u}{V}C_B + k_1 C_A - k_2 C_B \tag{33}$$

$$\frac{dT}{dt} = \frac{1}{\rho c_P}[k_1 e^{-E_1/RT} C_A(-\Delta H_1) + k_2 e^{-E_2/RT} C_B(-\Delta H_2) + k_3 e^{-E_3/RT} {C_A}^2(-\Delta H_3)] + \frac{u}{V}(T_{Feed} - T) + \frac{Q}{\rho c_P V} \tag{34}$$

$$y_1 = C_B \tag{35}$$

$$y_2 = T \tag{36}$$

The system has one controlled variable, which is the feed flow rate u, and both the concentration of B and the reactor temperature are measured, resulting in a MIMO system. The parameters for this problem are given in Table 3.

This system is simulated at two different operating points as investigated by Stack and Doyle.[14] The first one, denoted by point A, should not result in as severe nonlinearities as operating point B.[14] The operating conditions for those two points are summarized in Table 4.

A step size of 0.0002 h and q equal to 5000 were chosen for the computation of the empirical gramians. One hour of the process is simulated for varying initial/

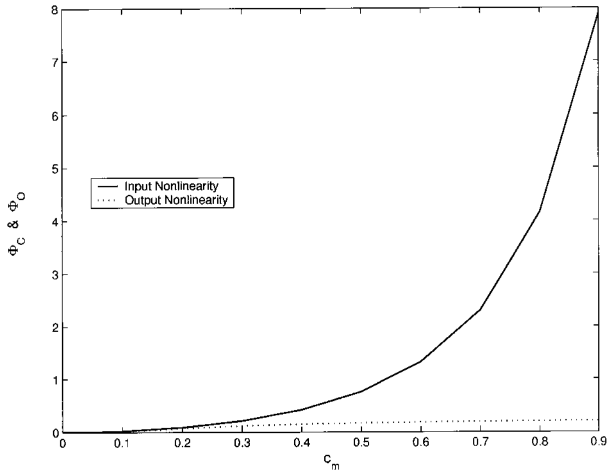

Figure 3. Input and output nonlinearity measures for operating point A.

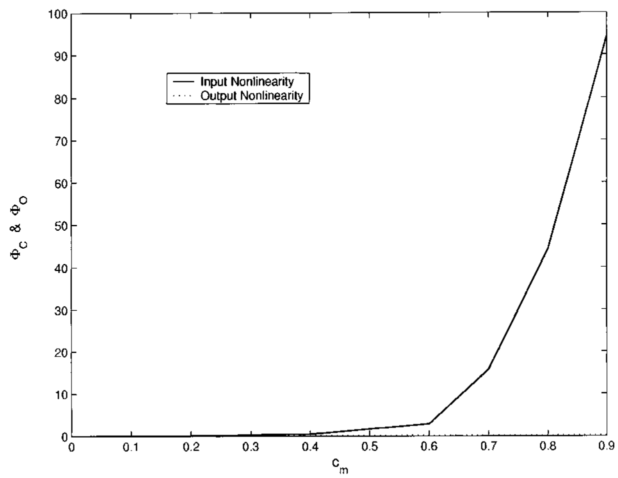

Figure 4. Input and output nonlinearity measures for operating point B.

input conditions, and the process will settle within this time for each simulation. It can be concluded from Figures 3 and 4 that the input–output behavior of these systems strongly deviates from the behavior of the linearized systems. Most of the nonlinearity occurs in the input-to-state behavior, because the input nonlinearity measure reaches a value of 8 for case A and 94 for case B for deviations of 90% in the input of the system. Since a value of close to unity in the nonlinearity measure can be considered a severe nonlinearity, the input-to-state behavior is very different from the linearized system. The state-to-output behavior exhibits only small deviations from the linearized system for both operating point A and operating point B over a large range of perturbations. Since the output-to-state behavior is very similar for both cases, but the system at operating point B exhibits more severe input nonlinearities than at operating point A, it can be concluded that the input–output behavior of the system is more nonlinear at point B. This behavior was predicted by Stack and Doyle[14] and is validated using their nonlinearity measure as well. This system can be classified as a Hammerstein-like process. It should be noted that the system at operating point A exhibits mildly nonlinear behavior over a wide operating region. However, the closer the system moves to the point of maximum conversion, the more nonlinear the system becomes, until it exhibits severe nonlinearities.

The results obtained with this method are in good agreement with results other researchers have found with their methods.[7,13,14] The advantage that this approach has over other nonlinearity measures is 3-fold. One is that independent results are given for the observability and controllability nonlinearity and based upon these the model can be classified according to section 3.4. The second advantage is that if model reduction needs to be performed on the model for online application, the results of the empirical gramians can be used.[2,3] A third advantage is that, after the computation of the empirical gramians, the nonlinearity measure is very easy to implement and does not require excessive computation time. Even when the computation of the empirical gramians is included, the method requires only a few seconds up to a few minutes, depending on the size of the model, to assess the nonlinearities. A disadvantage of this method compared to other approaches[8] is that there might exist a better linear model than the one computed from linearization at the operating point. If this case occurs, then this will be interpreted as process nonlinearity because it is a deviation from the behavior at the operating point.

5. Conclusions

This paper presents a new approach for nonlinearity assessment of control-affine models. The proposed measures are based upon the comparisons of the controllability and observability gramian with discrete empirical gramians based upon data collected within the operating region of the process. Large deviations between the controllability gramian and its empirical counterpart indicate nonlinearity in the input-to-state behavior. Differences between the observability gramian and its empirical counterpart can be found for models that exhibit nonlinear state-to-output behavior. Both measures must be taken into account to assess the input–output behavior of a system, as it is important for most controller design problems as well as model reduction. Based upon the two nonlinearity measures, systems can be classified as belonging to one of four categories for a specific operating region. These categories consist of mildly nonlinear systems, Wiener-like models, Hammerstein-like models, and models that are nonlinear in both input-to-state and state-to-output behavior. The measures developed here were applied to several examples from the literature on nonlinearity quantification, and the results were in good agreement with existing measures.

Literature Cited

(1) Henson, M. A.; Seborg, D. E. *Nonlinear Process Control*; Prentice Hall: Englewood Cliffs, NJ, 1997.

(2) Hahn, J.; Edgar, T. F. An Improved Approach to the Reduction of Nonlinear Models Using Balancing of Empirical Gramians. Submitted for publication in *Comput. Chem. Eng.*

(3) Hahn, J.; Edgar, T. F. A Balancing Approach to Minimal Realization and Model Reduction of Nonlinear Systems. Submitted for publication in *Ind. Eng. Chem. Res.*

(4) Desoer, C. A.; Wang, Y. T. Foundations of feedback theory for nonlinear dynamical systems. *IEEE Trans. Circuits Syst.* **1981**, *CAS-27* (2), 104.

(5) Haber, R. Nonlinearity test for dynamic processes. *Proceedings IFAC Identification and System Parameter Estimation Symposium, York, UK*; 1985; p 409.

(6) Nikolaou, M. When is Nonlinear Dynamic Modeling Necessary? *Proceedings of the 1993 ACC, San Francisco, CA*; 1993; p 910.

(7) Nikolaou, M.; Hanagandi, V. Nonlinearity Quantification and its Application to Nonlinear System Identification. *Chem. Eng. Commun.* **1998**, *166*, 1.

(8) Allgöwer, F. Definition and Computation of a Nonlinearity Measure. *Proceedings NOLCOS'95*; Pergamon: Oxford, UK, 1996; p 257.

(9) Helbig, A.; Marquardt, W.; Allgöwer, F. Nonlinearity Measures: Definition, Computation and Applications. *J. Process Control* **2000**, *10*, 113.

(10) Guay, M.; McLellan, P. J.; Bacon, D. W. Measurement of Nonlinearity in Chemical Process Control Systems: The Steady State Map. *Can. J. Chem. Eng.* **1995**, *73*, 868.

(11) Guay, M.; McLellan, P. J.; Bacon, D. W. Measurement Dynamic Process Nonlinearity. *Proc. IFAC Symposium ADCHEM'97, Banff, Canada*; 1997; p 589.

(12) Sun, D.; Hoo, K. A. Nonlinearity Measures for a Class of SISO Nonlinear Systems. *Int. J. Control* **2000**, *73*, 29.

(13) Harris, K. R.; Colantonio, M. C.; Palazoglu, A. On the Computation of a Nonlinearity Measure using Functional Expansions. *Chem. Eng. Sci.* **2000**, *55*, 2393.

(14) Stack, A. J.; Doyle III, F. J. Application of a Control-Law Nonlinearity Measure to the Chemical Reactor Analysis. *AIChE J.* **1997**, *43*, 425.

(15) Stack, A. J.; Doyle III, F. J. The Optimal Control Structure: An Approach to Measuring Control-Law Nonlinearity. *Comput. Chem. Eng.* **1997**, *21*, 1009.

(16) Carter (Ed.), G. C. *Coherence and time delay estimation*; IEEE Press: New York, 1993.

(17) Lall, S.; Marsden, J. E.; Glavaski, S. Empirical model reduction of controlled nonlinear systems. *14th IFAC World Congress, Beijing, China*; 1999.

(18) Lall, S.; Marsden, J. E.; Glavaski, S. A subspace approach to balanced truncation for model reduction of nonlinear control systems. Submitted for publication in *Int. J. Robust Nonlinear Control*.

(19) Zhou, K.; Doyle, J. C. *Essentials of Robust Control*; Prentice Hall: Englewood Cliffs, NJ, 1998.

(20) Moore, B. C. Principal component analysis in linear systems: controllability, observability, and model reduction. *IEEE Trans. Automat. Control* **1981**, *26*, 17.

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