Generalized Empirical Gramians for Trajectory Relevant Nonlinear Model Reduction *

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Abstract

In this paper we present a generalization of empirical gramians as used for nonlinear model reduction. This approach enables us to directly use data, generated by relevant trajectories, to compute the empirical controllability gramian. The observability gramian can be derived along the trajectory while ensuring that the perturbed initial conditions remain feasible. The feasibility of the perturbed initial conditions was an issue has not been discussed in literature. The reduction method is demonstrated on a plant with reactor and distillation unit with a recycle and base control. The model represents dynamics of class of real processes an is therefore more relevant than a case study on one single unit operation.

Keywords: nonlinear model reduction, empirical gramian, balancing

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1 Introduction

In process industry models that are available for optimization based control are not suitable for online applications. The dynamic optimization problem can not be solved within an acceptable time interval. Empirical gramians can be used to derive reduced order model by projection that can contribute in the solution of this problem. Although these projected models in general do not reduce the computational effort for numerical integration, it still can contribute in other steps in the optimization procedure.

Empirical gramians can be computed from data generated by simulations. Based upon these gramians we can distinguish between a relevant and an irrelevant subspace. By projection of the original model we can construct a reduced order model that represents the original model in its relevant dynamics. In case the data is generated by a linear model the empirical gramians coincide with the analytical solution. For the empirical gramians for nonlinear models we cannot check the result with a analytical solution since such a solution does not exist. We will show that these generalized empirical gramians provide suitable projections for nonlinear model reduction.

In process industry it is common to think in unit operations. Complete plants are build by connecting unit operations. The smallest plant that is rich enough to represents a large class of plants is a reaction unit connected to a separation unit with a recycle stream from separation to the reaction unit. This recycle stream is of crucial importance because the interconnected units exhibit completely different dynamics (Luyben *et al.*, 1999) than the separate unit operations. Since the results of nonlinear model reduction can be very problem specific we need to test techniques upon models that represent the fundamental characteristics of a real process. Base control should be considered as part of the plant since it will always be active during operation and effects the dynamics of the process. Nonlinear model reduction techniques should therefore be tested on a plant model including base control.

In this paper we well show how to derive reduced order models suitable to mimic the plant behaviour revealed by an optimal trajectory.

2 Nonlinear model reduction

In this paper we will focus on reduction of the number of differential equations. Two distinct phenomena can lead to a reduction of the number of differential equations. The presence of different time scales (Kokotovic *et al.*, 1986) can motivate a reduction by a suitable quasi steady state assumption (residualization or singular perturbation). Physical insight of the process does not always reveal which distinct differential equations cause two time scales. Tatrai *et al.* (1994a, 1994b) presented a state-eigenvalue association technique to distinguish between fast and slow differential equations. This technique was further explored by Robertson and Cameron (1997a, 1997b) and demonstrated on fairly large scale models with different unit operations and recycles. Since the state-eigenvalue association was done in the physical coordinates the sparsity of the model remains unchanged.

Weak input-output coupling is the second fundamental model motivation for model reduction. In control theory this is formalized in the controllability and observability properties of a model. For linear models the technique that provides a reduced order model by truncation is balanced reduction (Moore, 1981). The controllability and observability gramians that give rise to the proper coordinates for model reduction can be calculated from Lyapunov equations for stable linear models (e.g. Zhou, 1995). For nonlinear models reduction the empirical gramians were introduced by Lall (1998) and further explored by Hahn *et al.* (2000). Similar to the linear case the reduced model is derived by transformation and truncation of the original differential equations. This implies in general complete loss of sparsity of the differential part of the model and explains why this approach does not necessarily reduce computational effort. Scherpen (1993) presented a nonlinear extension of the linear gramians but are not feasible for large scale models. Lee *et al.* (2000) introduced a balanced projection based on subspace identification.

Proper Orthogonal Decomposition (POD) also called Karhunen-Loeve expansion or method of empirical eigenfunctions explores the weakly input to state coupling. Berkooz et al. (1993) presented in a review paper on POD a historical perspective of this research area. Successful applications of POD were presented in several papers e.g. Aling *et al.* (1996), Shvartsman *et al.* (2000), Theodoropoulou *et al.* (1998) and Banks (2000).

A more complete review on nonlinear model reduction techniques was given by Marquardt (2001).

3 Linear model reduction by projection

Since most nonlinear reduction approaches are extensions of the linear case we will first present a brief summary of relevant linear model reduction techniques.

Linear model reduction utilizes some transformation that provides a proper coordinate system for the reduction step. This coordinate change can either be based on some time scale separation or the notion of weak input-output coupling. In the coordinate system where slow and fast dynamics can be separated the appropriate reduction is achieved by residualization. In the coordinate system where the strong and weakly coupled dynamics can be separated reduction is achieved by truncation. In this paper we will not consider the transformation that provides the separation in fast and slow dynamics but we consider the separation in strong and weakly coupled dynamics. Weakly coupled dynamics is the part of the system that is badly controllable and observable. Balancing the controllable and observable dynamics of a system distinguishes between the strongly coupled dynamics and the weakly coupled dynamics. This enables us to find the dominant dynamics for the input-output behaviour of the system.

3.1 Balancing linear systems

Balancing of linear systems has been first presented by Moore (1981). Let us define a stable linear time invariant system

$$\begin{bmatrix} \dot{x} \\ y \end{bmatrix} = \left[\begin{array}{c|c} A & B \\ \hline C & D \end{array}\right] \begin{bmatrix} x \\ u \end{bmatrix} \tag{1}$$

P and Q are respectively the controllability and observability gramians of system (1) such that

$$AP + PA^T + BB^T = 0 \tag{2}$$
$$QA + A^TQ + C^TC = 0 \tag{3}$$

This is a balanced realization iff

$$P = Q = \Sigma \tag{4}$$

with Σ diagonal and $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$. If the system is not a balanced realization there exists a transformation T after which the transformed system is a balanced realization. In text books (e.g. Zhou, 1995) different approaches can be found to calculate T.

For a stable linear discrete time system

$$\begin{bmatrix} x_{k+1} \\ y_k \end{bmatrix} = \left[\begin{array}{c|c} F & G \\ \hline C & D \end{array}\right] \begin{bmatrix} x_k \\ u_k \end{bmatrix} \tag{5}$$

W_c and W_o are respectively the discrete time controllability and observability gramians of system (5) such that

$$\begin{aligned} FW_cF^T - W_c + GG^T = 0 \\ F^TW_oF - W_o + C^TC = 0 \end{aligned} \tag{6}$$

or in recursive form and finite time

$$W_c^{k+1} = F W_c^k F^T + G G^T, \quad W_c^k = \sum_{n=0}^{k} F^n B B^T F^{T^n} \tag{7}$$

$$W_o^{k+1} = F^T W_o^k F + C^T C, \quad W_o^k = \sum_{n=0}^{k} F^{T^n} C^T C F^n \tag{8}$$

Similar to the continuous time system the discrete time system is a balanced realization iff

$$W_c = W_o = \Sigma \tag{9}$$

with Σ diagonal and $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$.

3.2 Reduction by truncation or residualization

In general we can reduce a linear model that is arranged in a suitable coordinate system

$$\begin{bmatrix} \dot{z}_1 \\ \dot{z}_2 \\ y \end{bmatrix} = \left[\begin{array}{cc|c} A_{11} & A_{12} & B_1 \\ A_{21} & A_{22} & B_2 \\ \hline C_1 & C_2 & D \end{array}\right] \begin{bmatrix} z_1 \\ z_2 \\ u \end{bmatrix} \tag{10}$$

by truncation: $z_2 = 0$ ($\Rightarrow \dot{z}_2 = 0$)

$$\begin{bmatrix} \dot{z}_1 \\ y \end{bmatrix} = \left[\begin{array}{c|c} A_{11} & B_1 \\ \hline C_1 & D \end{array}\right] \begin{bmatrix} z_1 \\ u \end{bmatrix} \tag{11}$$

or residualization: $\dot{z}_2 = 0$

$$\begin{bmatrix} \dot{z}_1 \\ 0 \\ y \end{bmatrix} = \left[\begin{array}{cc|c} A_{11} & A_{12} & B_1 \\ A_{21} & A_{22} & B_2 \\ \hline C_1 & C_2 & D \end{array}\right] \begin{bmatrix} z_1 \\ z_2 \\ u \end{bmatrix} \tag{12}$$

which results in a set of linear differential algebraic equations from which z_2 can be eliminated

$$\begin{bmatrix} \dot{z}_1 \\ y \end{bmatrix} = \left[\begin{array}{c|c} A_{11} - A_{12}A_{22}^{-1}A_{21} & B_1 - A_{12}A_{22}^{-1}B_2 \\ \hline C_1 - C_2A_{22}^{-1}A_{21} & D - C_2A_{22}^{-1}B_2 \end{array}\right] \begin{bmatrix} z_1 \\ u \end{bmatrix} \tag{13}$$

Both reductions are projections: in case of truncation a complete subspace is projected onto zero and in case of residualization the dynamics is projected onto a subspace. Note that truncation is a special case of residualization.

4 Nonlinear model reduction by projection

A large class of nonlinear models can be described by a set of explicit differential and algebraic equations

$$\begin{aligned} \dot{x} &= f(x, y, u) \\ 0 &= g(x, y, u) \end{aligned} \tag{14}$$

where x, y and u are state, algebraic and input variables of suitable dimension, respectively. Nonlinear models can be reduced by projection similarly to linear case with the same distinction between truncation and residualization. In general we first need to transform to a new coordinate system that is suitable for model reduction. For the nonlinear case is is favorable to transform after subtraction of a (preferably) steady state value or some average value

$$z = T(x - x_0) \Leftrightarrow x = x_0 + T^{-1}z \tag{15}$$

Differentiation z and substitution of the original differential and algebraic equations yields

$$\begin{array}{rcr} \dot{z} &=& Tf(x_0 + T^{-1}z, y, u) \\ 0 &=& g(x_0 + T^{-1}z, y, u) \end{array} \tag{16}$$

We now can distinguish two complementary subspaces for model reduction (note the abuse of notation of T_1^{-1} and T_2^{-1})

$$\begin{bmatrix} z_1 \\ z_2 \end{bmatrix} = \begin{bmatrix} T_1 \\ T_2 \end{bmatrix} (x - x_0) \Leftrightarrow x = x_0 + \begin{bmatrix} T_1^{-1} & T_2^{-1} \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} \tag{17}$$

Similar to the linear case we now can reduce the model by truncation ($z_2 = 0$)

$$\begin{array}{rcr} \dot{z}_1 &=& T_1 f(x_0 + T_1^{-1}z_1, y, u) \\ 0 &=& g(x_0 + T_1^{-1}z_1, u, u) \end{array} \tag{18}$$

Like in the linear case truncation reduces the total number of equations by a reduction of differential equations. Residualization of a nonlinear model yields ($\dot{z}_2 = 0$)

$$\begin{array}{rcr} \dot{z}_1 &=& T_1 f(x_0 + T^{-1}z, y, u) \\ 0 &=& T_2 f(x_0 + T^{-1}z, y, u) \\ 0 &=& g(x_0 + T^{-1}z, u, u) \end{array} \tag{19}$$

Note that in general z_2 can not be eliminated as in the linear case. Therefore residualization of a nonlinear model only reduces the number of differential equations but does not reduce the total number of equations.

5 Empirical Gramians

In the linear case the controllability and observability are calculated by solving two Lyapunov equations. For nonlinear models these Lyapunov equations are not defined but we can derive empirical gramians introduced by Lall (1999, 2002). For linear models these empirical gramians coincide with the analytical solutions of the Lyapunov equations (3) or discrete time Lyapunov equations (6). The following sets need to be defined for empirical input gramian:

$$
\begin{aligned}
T^n &= \{T_1, \ldots, T_r \mid T_l \in \mathbb{R}^{n\times n}, T_l T_l^T = I, l = 1, \ldots, r\} & (20)\\
M &= \{c_1, \ldots, c_s \mid c_m \in \mathbb{R}^+, m = 1, \ldots, s\} & (21)\\
E^n &= \{e_1, \ldots, e_n \mid \text{standard unit vectors in } \mathbb{R}^n\} & (22)
\end{aligned}
$$

where r is the number of different perturbation orientations, s is the number of different perturbation magnitudes and n is the number of inputs of the system for the controllability gramian and the number of states of the full order system for the observability gramian. The empirical controllability and observability gramian as defined by Lall:

Empirical controllability gramian. Let T^p, M and E^p be given as described above, where p is the number of inputs of the system. The empirical controllability gramian for system (1) is defined by

$$P = \sum_{l=1}^{r}\sum_{m=1}^{s}\sum_{i=1}^{p} \frac{1}{rsc_m^2}\int_0^\infty \Phi^{ilm}(t)dt \tag{23}$$

where $\Phi^{ilm}(t) \in \mathbb{R}^{n\times n}$ is given by

$$\Phi^{ilm}(t) := (x^{ilm}(t) - x_{ss})(x^{ilm}(t) - x_{ss})^T \tag{24}$$

and $x^{ilm}(t)$ is the state of the system corresponding to the impulsive response $u(t) = c_m T_l e_i \delta(t) + u_{ss}$ with initial condition $x_0 = x_{ss}$.

Empirical observability gramian. Let T^n, M and E^n be given as described above, where n is the number of states of the original system. The empirical observability gramian for system (1) is defined by

$$Q = \sum_{l=1}^{r}\sum_{m=1}^{s} \frac{1}{rsc_m^2}\int_0^\infty T_l \Psi^{lm}(t) T_l^T dt \tag{25}$$

where $\Psi^{lm}(t) \in \mathbb{R}^{n\times n}$ is given by

$$\Phi_{ij}^{ilm}(t) := (y^{ilm}(t) - y_{ss})^T (y^{jlm}(t) - y_{ss}) \tag{26}$$

and $y^{ilm}(t)$ is the output of the system corresponding to the initial condition $x_0 = c_m T_l e_i + x_{ss}$ and input $u(t) = u_{ss}$.

Discrete time empirical controllability gramian. Let T^p, M and E^p be given as described above, where p is the number of inputs of the system. The discrete time empirical controllability gramian for system (5) is defined by

$$W_c = \sum_{l=1}^{r} \sum_{m=1}^{s} \sum_{i=1}^{p} \frac{1}{rsc_m^2} \sum_{k=0}^{q} \Phi_k^{ilm} \tag{27}$$

where $\Phi_k^{ilm} \in \mathbb{R}^{n \times n}$ is given by

$$\Phi_k^{ilm}(t) := (x_k^{ilm} - x_{ss})(x_k^{ilm} - x_{ss})^T \tag{28}$$

and x_k^{ilm} is the state of the system corresponding to the impulsive response $u_k = c_m T_l e_i \delta_{k=0} + u_{ss}$ with initial condition $x_0 = x_{ss}$.

Discrete time empirical observability gramian. Let T^n, M and E^n be given as described above, where n is the number of states of the original system. The discrete time empirical observability gramian for system (5) is defined by

$$W_o = \sum_{l=1}^{r} \sum_{m=1}^{s} \frac{1}{rsc_m^2} \sum_{k=0}^{q} T_l \Psi_k^{lm} T_l^T \tag{29}$$

where $\Psi_k^{lm} \in \mathbb{R}^{n \times n}$ is given by

$$\Phi_{ij}^{ilm}{}_k := (y_k^{ilm} - y_{ss})^T (y_k^{jlm} - y_{ss}) \tag{30}$$

and y_k^{ilm} is the output of the system corresponding to the initial condition $x_0 = c_m T_l e_i + x_{ss}$ and input $u_k = u_{ss}$.

6 Generalized empirical gramians

We will now propose a generalization of the discrete time empirical gramians.

Let $u(k) \in \mathbb{R}^r$ be an arbitrary but relevant input sequence

$$u(k) = [u_0, u_1, \ldots, u_k, \ldots, u_{N-1}] \tag{31}$$

where p in the number of inputs of the system and N is the number of samples. The state response $x(k) \in \mathbb{R}^n$ is

$$x(k) = [x_1, \ldots, x_k, \ldots, x_N] \tag{32}$$

where n is the number of states of the original system and N is the number of samples.

Define the data matrix $X_N \in \mathbb{R}^{n\times N}$ as

$$X_N = [\bar{x}_1|\dots|\bar{x}_k|\dots|\bar{x}_N] \tag{33}$$

where $\bar{x}_k = x_k - x_{ss}$ and input matrix $U_N \in \mathbb{R}^{(q+1)\times N}$

$$U_N = \begin{bmatrix} \bar{u}_0 & \bar{u}_1 & \dots & \bar{u}_q & \dots & \bar{u}_{N-1} \\ 0 & \bar{u}_0 & \dots & \bar{u}_{q-1} & & \\ \vdots & \ddots & \ddots & \vdots & & \vdots \\ 0 & \dots & 0 & \bar{u}_0 & \dots & \bar{u}_{N-1-q} \end{bmatrix} \tag{34}$$

where $\bar{u}_k = u_k - u_{ss}$ and q is the number of samples that is chosen such that the relevant slow dynamics are present in the data.

Discrete time empirical controllability gramian. Let U_N and X_N be given as described above. The discrete time empirical controllability gramian for system (5) is defined by

$$W_c = X_N U_N^{\dagger} {U_N^{\dagger}}^T X_N^T \tag{35}$$

where $U_N^{\dagger} \in \mathbb{R}^{N\times n}$ is right inverse of U_N

$$U_N^{\dagger} = U_N^T (U_N U_N^T)^{-1}$$

Proof: The data matrix X_N can be written as

$$X_N = \Gamma_c U_N \tag{36}$$

with controllability matrix

$$\Gamma_c = \begin{bmatrix} G & FG & \dots & F^q G \end{bmatrix} \tag{37}$$

therefore

$$X_N U_N^{\dagger} {U_N^{\dagger}}^T X_N^T = \Gamma_c U_N U_N^{\dagger} {U_N^{\dagger}}^T U_N^T \Gamma_c^T = \Gamma_c \Gamma_c^T = W_c \tag{38}$$

which is a solution of the recursive discrete time Lyapunov equation (7).

Let us define a set of N arbitrary perturbations on initial conditions $X_0 \in \mathbb{R}^{n\times N}$

$$X_0 = \begin{bmatrix} x_0^1 & x_0^2 & \dots & x_0^N \end{bmatrix} \tag{39}$$

where n is the number of states of the original system. Let $y^i(k) \in \mathbb{R}^h$ where h is the number of outputs

$$y^i(k) = \left[y_1^j, \ldots, y_k^j, \ldots, y_q^j\right] \tag{40}$$

be the response of the system with initial condition $x(0) = x_0^j + x_{ss}$ and input $u(k) = u_{ss}$.

Let us define a data matrix Y_N

$$Y_N = \begin{bmatrix} \bar{y}_0^1 & \bar{y}_0^2 & \ldots & \bar{y}_0^N \\ \bar{y}_1^1 & \bar{y}_1^2 & \ldots & \bar{y}_1^N \\ \vdots & & & \vdots \\ \bar{y}_q^1 & \bar{y}_q^2 & \ldots & \bar{y}_q^N \end{bmatrix} \tag{41}$$

where $\bar{y}_k^j = y_k^j - y_{ss}$.

Discrete time empirical observability gramian. Let X_0 and Y_N be given as described above. The discrete time empirical observability gramian for system (5) is defined by

$$W_o = X_0^{\dagger T} Y_N^T Y_N X_0^\dagger \tag{42}$$

where $X_0^\dagger \in \mathbb{R}^{N \times n}$ is the right inverse of X_0

$$X_0^\dagger = X_0^T (X_0 X_0^T)^{-1} \tag{43}$$

where q is the number of samples that is chosen such that the system reaches a steady state at $k < q$ for all any kind of initial condition response.

Proof: The data matrix Y_N can be written as

$$Y_N = \Gamma_o X_0 \tag{44}$$

with the truncated observability matrix

$$\Gamma_c = \begin{bmatrix} C \\ CF \\ \vdots \\ CF^q \end{bmatrix} \tag{45}$$

therefore

$$X_0^{\dagger T} Y_N^T Y_N X_0^\dagger = X_0^{\dagger T} X_0^T \Gamma_o^T \Gamma_o X_0 X_0^\dagger = \Gamma_o^T \Gamma_o = W_o \tag{46}$$

which is a solution of the recursive discrete time Lyapunov equation (8).

This definition of empirical gramians is more general since the only condition on the data is that the right inverses $U_N^\dagger$ and $X_0^\dagger$ should exist. The class of admissible input signals and initial condition perturbation is not as restrictive as for the empirical gramians as defined by Lall (1999).

7 Example: CSTR with exothermic reaction

The relevance of the generalization presented in the previous section can be demonstrated on a simple example.

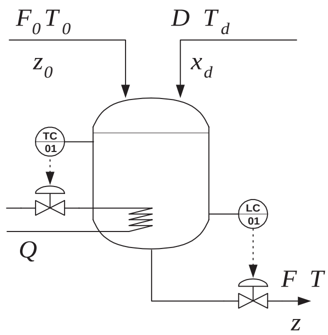

Figure 1: CSTR with first order exothermic reaction

The example is a simple continuous stirred tank reactor with an first order exothermic reaction $A \rightarrow B$. A proportional level and temperature controller are added to stabilize the process as depicted in Figure 1. Typically F_0 is a fresh feed and D is a recycling stream from a downstream separation section.

In this particular example we want to calculate controllability and observability of the process. Therefore we need to define inputs and outputs. Since the process is already stabilized by proportional controllers we will consider the set-points as the new inputs: $\texttt{SP}_{\texttt{LC.01}}$ and $\texttt{SP}_{\texttt{TC.01}}$. As outputs we choose overall molar holdup N and temperature T. Since the process is most likely operated optimal at its constraints we want to generate data near this operating area. This is depicted in Figure 2. If some other specific sequence is favorable this can be chosen freely.

The state trajectories corresponding to these inputs are shown in Figure 3. Figures (2) and (3) contain the information from which the empirical

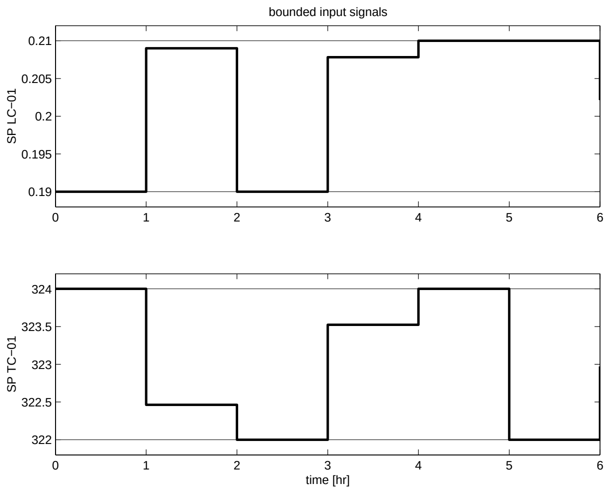

Figure 2: Input signals used for data generation

controllability gramian can be derived by Equation (35). In order to judge the numerical values of the empirical gramian we can derive a linear model and compare solution of the discrete time controllability Lyapunov Equation (6). Furthermore we can interchange the nonlinear model with the linearized model and derive the empirical gramian again. This result compared with the solution from the Lyapunov equation shows the quality of procedure to derive the empirical gramian. Comparing the numerical values we can see

$$
\begin{array}{cc}
\text{Lyapunov} & \begin{bmatrix} 7.4860 \cdot 10^{-2} & -2.2155 \cdot 10^{-5} & 1.1486 \cdot 10^{-3} \\ -2.2155 \cdot 10^{-5} & 2.9961 \cdot 10^{-5} & -1.4790 \cdot 10^{-3} \\ 1.1486 \cdot 10^{-3} & -1.4790 \cdot 10^{-3} & 6.4974 \cdot 10^{-1} \end{bmatrix} \\
\\
\text{Empirical Linear} & \begin{bmatrix} 7.4855 \cdot 10^{-2} & -2.2164 \cdot 10^{-5} & 1.1427 \cdot 10^{-3} \\ -2.2164 \cdot 10^{-5} & 2.9961 \cdot 10^{-5} & -1.4790 \cdot 10^{-3} \\ 1.1427 \cdot 10^{-3} & -1.4790 \cdot 10^{-3} & 6.4969 \cdot 10^{-1} \end{bmatrix} \\
\\
\text{Empirical Nonlinear} & \begin{bmatrix} 7.4855 \cdot 10^{-2} & -2.0386 \cdot 10^{-5} & 1.1177 \cdot 10^{-3} \\ -2.0386 \cdot 10^{-5} & 3.0420 \cdot 10^{-5} & -1.5311 \cdot 10^{-3} \\ 1.1177 \cdot 10^{-3} & -1.5311 \cdot 10^{-3} & 6.5694 \cdot 10^{-1} \end{bmatrix}
\end{array}
$$

Table 1: Controllability gramians

that the empirical gramian or the linear model is a good approximation of the solution of the Lyapunov solution. This implies that the method indeed can reproduce the controllability gramian. The empirical controllability gramian

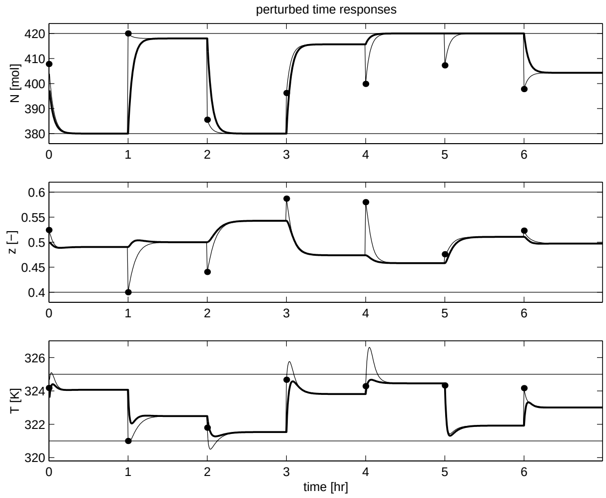

Figure 3: Responses of the system to input sequence and perturbed initial conditions (dots)

of the nonlinear model is slightly different from the empirical gramian of the linear model which suggest some minor nonlinear behaviour.

For the empirical observability gramian we will use the same input data as for the controllability gramian. So this data was close to the constraints of the process. Since the interval between two different inputs was long enough to reach a new steady state we can use the previous simulations to retrieve perturbed initial condition responses. These perturbed initial conditions are show with the dots in Figure 3 and will be further explained by Figure 4 which is a detail of Figure 3. It that shows the response of a set point change for both the molar holdup as well for the temperature. The inputs do not change from $2 \leq t < 3$. We now can define $x_0^2 = x(2)$, $x_{ss}^2 = x(3)$ and $u_{ss}^2 = u(3)$ with its initial condition response $\bar{y}^2(t) = y(t+2) - y_{ss}^2$. In case that the system is not controllable the collection of initial conditions does not span the whole state space and therefore the right inverse as defined in Equation (43) does not exist. We can easily deal with this by adding a perturbation to the initial condition. This implies that we need to do new simulations with the perturbed initial conditions. In this case we have a nearly uncontrollable system and therefore we have to add this extra perturbation to the initial condition. The original and the perturbed simulation results are shown in Figure (3) with the solid and dotted line respectively.

Again we want will compare the empirical gramian for the nonlinear model to the result of the empirical gramian of the linear model and the

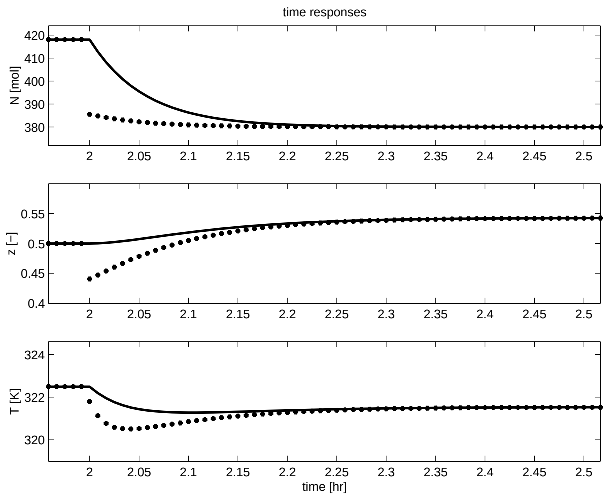

Figure 4: Detail with original (solid line) and perturbed initial condition (dotted line)

solution of the Lyapunov Equation (6) that can be solved based on the linear model system matrices. In this setting it is also easy to deal with constraints

Lyapunov	$\begin{bmatrix} 3.8594 \cdot 10^0 & 1.1850 \cdot 10^0 & 1.8250 \cdot 10^{-2} \\ 1.1850 \cdot 10^0 & 2.0052 \cdot 10^3 & 1.5071 \cdot 10^1 \\ 1.8250 \cdot 10^{-2} & 1.5071 \cdot 10^1 & 1.7400 \cdot 10^0 \end{bmatrix}$
Empirical Linear	$\begin{bmatrix} 3.8597 \cdot 10^0 & 1.1901 \cdot 10^0 & 1.8457 \cdot 10^{-2} \\ 1.1901 \cdot 10^0 & 2.0052 \cdot 10^3 & 1.5074 \cdot 10^1 \\ 1.8457 \cdot 10^{-2} & 1.5074 \cdot 10^1 & 1.7401 \cdot 10^0 \end{bmatrix}$
Empirical Nonlinear	$\begin{bmatrix} 3.8606 \cdot 10^0 & 2.0178 \cdot 10^0 & 2.6687 \cdot 10^{-2} \\ 2.0178 \cdot 10^0 & 2.3923 \cdot 10^3 & 1.9589 \cdot 10^1 \\ 2.6687 \cdot 10^{-2} & 1.9589 \cdot 10^1 & 1.8162 \cdot 10^0 \end{bmatrix}$

Table 2: Observability gramians

on state variables. This is important since a perturbation of initial condition may result in a constraint violation or even in unfeasible values. This is typically the case for fractions such as the state variable z if close to zero or one. Adding a perturbation can result in negative values or values larger than one which are no feasible values for a fraction. This issue is not addressed in the papers by Lall or Hahn but has a large impact on the applicability of their Empirical Observability Gramian. We simply can constrain all initial conditions as shown in Figure 3, were the somewhat arbitrary constraints $395 \leq N \leq 405$, $321 \leq T \leq 325$ and $0.4 \leq z \leq 0.5$ were implemented just to show the principle.

This example is too small to demonstrate the value of the empirical gramians for model reduction. The purpose of this example was to show the principles of the method and that for the linear case the empirical gramians approximates the solution of the Lyapunov equations for controllability and observability. In order to demonstrate the value for model reduction we need al larger model and that will be presented in the next section.

8 Application: reaction separation process

In chemical process it is not attractive to operate a reactor such that the desired high quality product is produced at once. This can be explained by the fact that this production strategy would result in very large reactors and therefore in high investment costs. Therefore it is very common to combine a reactor unit with a separation unit where the high quality product is removed from the process and the low quality product is recycled into the reactor again. Investment costs related to this second production strategy are in

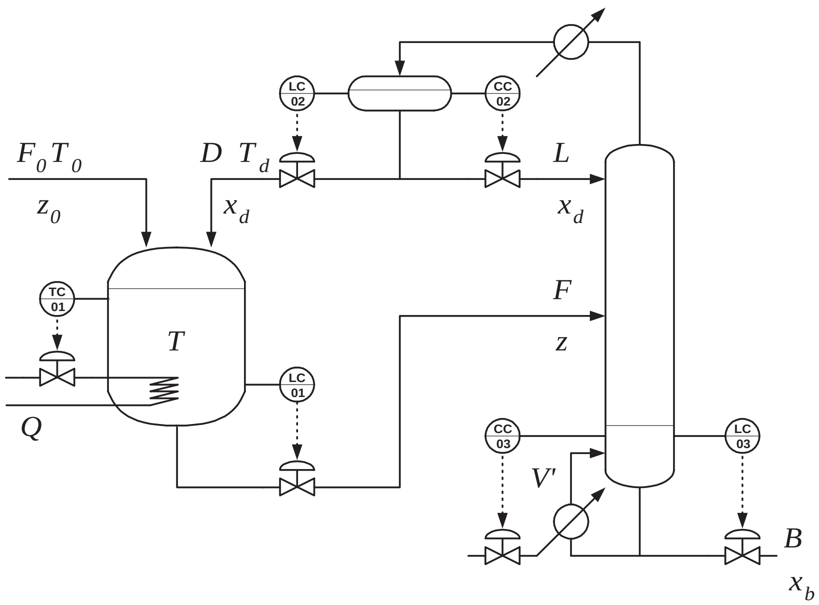

Figure 5: Reaction separation process

general much lower and therefore more common in industry. The recycle can be considered as a feedback and can have a large impact on the overall dynamics (e.g. Lyuben, 1999 or Wu, 1996) and makes a plant wide reduction strategy more favorable than a unit wise reduction strategy. This motivates the application to a reactor separation process with a recycle in this paper. The process flow sheet is depicted in Figure 5. The reactor that was used in the previous example is interconnected with a binary distillation column (Skogestad, 1997) resulting in a process with a recycle stream.

The plant is controlled by three level controllers, a temperature controller and two quality controllers. Typically quality measurements can be hard to obtain and are serious candidates to predict by a model. That motivates the choice for the three qualities as outputs. The plant is laid out with a push throughput control strategy which explains the choice of the fresh feed into the reactor as the input.

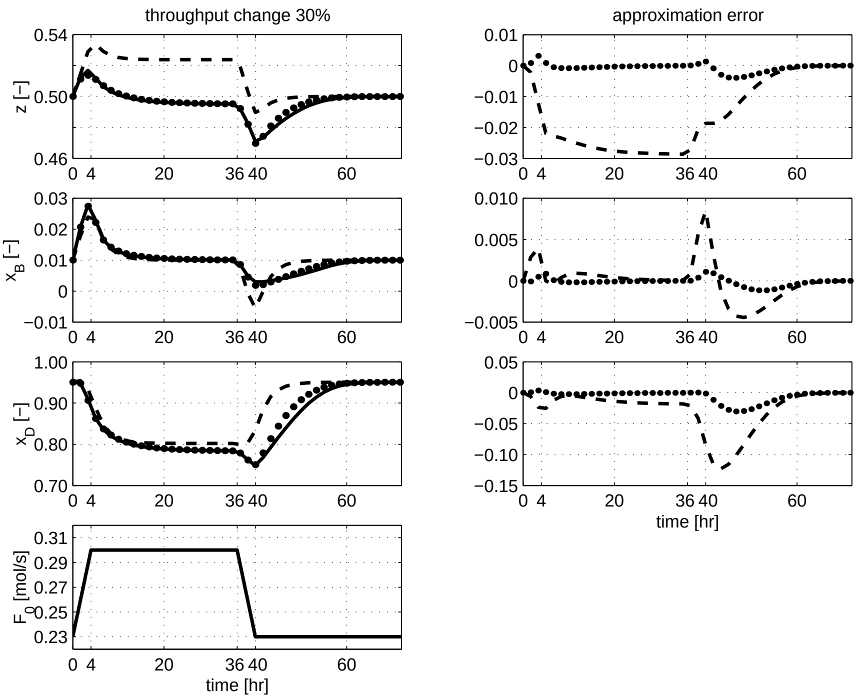

Figure 6: Throughput change of 30%. Original nonlinear (45^{th}order): solid. Reduced nonlinear (4^{th}order): dotted. Linear model (45^{th}order): dashed

The trajectory relevance of the method as applied here is that the model reduction is based on the desired trajectory that is known in advance. The operating envelop described by this trajectory is the envelop where the reduced model should perform with enough accuracy.

To demonstrate the reduction method we choose the fresh feed (F_0) of the reactor as an input and the quality in the reactor, and top and bottom quality in the column as outputs, respectively z, x_d and x_b. The relevant trajectory was defined as a increase of the input of 30% in 4 hours as depicted in the bottom left of Figure (6). Furthermore is shown in Figure (6) the responses of the original (45^{th}order) model, reduced (4^{th}order) model and a linear model. The linear model is added to reveal the nonlinear behaviour of the process.

9 Conclusion

In this paper we presented a generalization of the empirical gramians. In this generalized form we can directly use data generated by a relevant trajectory to construct the empirical gramians. Furthermore, we can assure that perturbed initial conditions that are used for the empirical observability gramian remain feasible. This problem was not addressed in the original setting of the empirical observability gramian.

The generalized empirical gramians were explained by computing them for a continuously stirred tank reactor. This example was too small to demonstrate model reduction and therefore it was also demonstrated on a plant with two unit operations and a recycle stream and base control. Such a model represents dynamics of a large class of real processes an is therefore more relevant than a case study on a single unit operation.

The original model with 45 differential equations could be reduced to a 4^{th} order model that still represents the input output behaviour for the ramped throughput change.

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