Data-driven nonlinear system identification of a closed-loop CSTR

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1. INTRODUCTION

Recently, data-driven system identification using sparse regression with L_1 regularisation solved the problem to identify simultaneously functional structure and the related parameter estimates [Brunton et al. (2016)]. Based on this open-loop framework, the objectives of this paper are to theoretically examine the performance of the data-driven nonlinear system identification using a sequential threshold least-squares (STLSQ) algorithm based on sparse regression with L_1 regularisation for closed-loop processes. Additionally, the effect of normalisation on the proposed method is discussed. In order to evaluate the method, a CSTR model with a PI controller to control the reactor temperature is chosen as benchmark system and the model is identified using the proposed framework. Finally, the validation of the proposed method using simulation results are presented.

2. SPARSE IDENTIFICATION OF NONLINEAR DYNAMICS

The sparse identification framework seeks to identify dynamic systems in the form of

$$\frac{dx(t)}{dt} = f(x(t)),\ x(t_0) = x_0, \tag{1}$$

describing the temporal behaviour of the state vector $x(t) \in \mathbb{R}^n$. Data-driven system identification consists of the identification of nonlinear candidates using the properties of dictionary learning and regularisation [Brunton et al. (2016)]. The resulting regression problem can be written as:

$$\min_{\Xi} \|\Theta(X) \cdot \Xi - \dot{X}\|_2 + \lambda \cdot \|\Xi\|_1. \tag{2}$$

where the output of the regression is the matrix $\Xi \in \mathbb{R}^{(\sum d_i) \times n}, i = 1, 2, .., H$, which contains the model coefficients for each candidate function from the dictionary function $\Theta(X)$ fit to the data matrix $X \in \mathbb{R}^{m \times n}$ and its derivative obtained from the process $\dot{X} \in \mathbb{R}^{m \times n}$. $\lambda \in \mathbb{R}$ denotes the regularisation parameter. In order to improve the optimisation performance, [Brunton et al. (2016), Wang et al. (2011)] recommend the normalisation of the dictionary function. The idea can be transferred to a closed-loop identification by adding a manipulated variable into the regression problem. Reformulating the regression problem in an augmented state-space form can account for PI controllers commonly used in practical applications. The resulting state-space form is

$$\frac{dx}{dt} = a(x) + K_p \cdot (w - y) + K_I \cdot z, \tag{3}$$

$$\frac{dz}{dt} = w - y, \tag{4}$$

$$y = x. \tag{5}$$

where $x \in \mathbb{R}$ is a single state, $y \in \mathbb{R}$ is the system output, $w \in \mathbb{R}$ is the reference value to which the system should be controlled, $z \in \mathbb{R}$ is the auxiliary state and $K_p \in \mathbb{R}$ and $K_I \in \mathbb{R}$ are, respectively, the proportional and integral gains.

3. SIMULATION AND RESULTS

In order to evaluate the performance of the proposed solution in a continuous time environment, a CSTR model was used. The state-space model consists of the mass balance, the energy balance and the PI controller structure. The nonlinear part of the model is represented by the reaction kinetics containing the Arrhenius equation. The model parameters are given in Table 1 and the model is

$$\begin{aligned}
\frac{dc_A}{dt} &= \frac{q}{V} \cdot (c_{Af} - c_A) - rA \\
\frac{dT}{dt} &= \frac{q}{V} \cdot (T_f - T) - \frac{\Delta H_R}{(\rho \cdot c_p)} \cdot rA + \\
&\quad \frac{U \cdot A}{(V \cdot \rho \cdot c_p)} \cdot (T_c - T) + PI \\
\frac{dz}{dt} &= T_{ref} - T \\
rA &= k_0 \cdot e^{-E/R \cdot T} \cdot c_A^2 \\
PI &= K_p \cdot (T_{ref} - T) + K_I \cdot z.
\end{aligned} \tag{6}$$

where $T \in \mathbb{R}$ is the reactor temperature, $c_A \in \mathbb{R}$ is the concentration of the considered component, $z \in \mathbb{R}$ describes the integrated control error state and $PI \in \mathbb{R}$ is the PI-controller structure. Parameters and initial conditions of the model are shown in Table 1.

The model equations were implemented and solved in Python to obtain data for the identification. The identification was performed with a threshold of $\lambda = 0.9$, ten iterations in the STLSQ algorithm, and a normalised dictionary. The resulting coefficient matrix containing the

	$\frac{dc_A}{dt}$	$\frac{dT}{dt}$	$\frac{dz}{dt}$	
1	20	$1.41 \cdot 10^4$	380	Other model coefficients
T	0	-37	-1	
c_A	-5	0	0	
z	0	180	0	PI controller
$T^2 \cdot e^{-E/R \cdot T}$	0	0	0	
$T^2 \cdot e^{-E/R \cdot c_A}$	0	0	0	Reaction kinetics
$c_A^2 \cdot e^{-E/R \cdot T}$	$-8.46 \cdot 10^6$	$4.21 \cdot 10^8$	0	
$c_A^2 \cdot e^{-E/R \cdot c_A}$	0	0	0	
$z^2 \cdot e^{-E/R \cdot T}$	0	0	0	
$z^2 \cdot e^{-E/R \cdot c_A}$	0	0	0	

Fig. 1. Result of sparse identification with nonlinear dynamics applied to the CSTR model with PI temperature controller described by Equation 6.

candidate functions as rows and the differential equations as columns is shown in Figure 1. It can be observed that the appropriate candidate functions representing the actual dynamics were identified and a sparse solution was obtained. The candidate functions and coefficients chosen by the identification are the same as specified in the input model (see Table 1). The coefficient of determination $R^2 = 1$ confirms that the resulting model is appropriate. To produce different dynamical responses of the model and evaluate the effect of normalisation, the initial conditions of the CSTR model with PI controller were randomly varied to produce 51 different data sets for identification. Figure 2 shows the number of nonzero coefficients in the identified model equations as a function of the initial conditions. When no normalisation is performed (red triangles), none of the models has the desired nine nonzero coefficients, while with normalisation (blue triangles), the desired model is found in most cases. It was shown that, with respect to the sparsity of the model, the normalisation has a significant effect and improves the identification. Furthermore, it is assumed that the normalisation of the dictionary improves the predictive capacity of the models.

Table 1. Parameters and initial conditions of the model

q	Volumetric Flowrate ($5\,\mathrm{m^3/h}$)
V	Reactor Volume ($1\,\mathrm{m^3}$)
ρ	Density of Mixture ($1000\,\mathrm{kg/m^3}$)
c_p	Heat Capacity of Mixture ($0.231\,\mathrm{kJ/(kg \cdot K)}$)
ΔH_R	Heat of Reaction ($-1.15 \cdot 10^4\,\mathrm{kJ/kmol}$)
E	Activation Energy ($50000\,\mathrm{kJ/kmol}$)
R	Gas Constant ($8.314\,\mathrm{kJ/(kmol \cdot K)}$)
k_0	Reaction Constant ($8.46 \cdot 10^6\,\mathrm{m^3/(kmol \cdot h)}$)
U	Heat Transfer Coeff. ($5000\,\mathrm{kJ/(m^3 \cdot h)}$)
A	Heat Transfer Area ($1\,\mathrm{m^3}$)
T_f	Feed Temperature ($350\,\mathrm{K}$)
c_{Af}	Feed Concentration Comp. A ($4\,\mathrm{kmol/m^3}$)
T_c	Cooling Jacket Temperature ($395\,\mathrm{K}$)
T_{ref}	Controller Reference Temperature ($380\,\mathrm{K}$)
K_p	Controller Proportional Gain ($10\,\mathrm{1/h}$)
K_I	Controller Integral Gain ($180\,\mathrm{1/h^2}$)
c_{A0}	Initial Concentration Comp. A ($2.2\,\mathrm{kmol/m^3}$)
T_0	Initial Temperature ($325\,\mathrm{K}$)

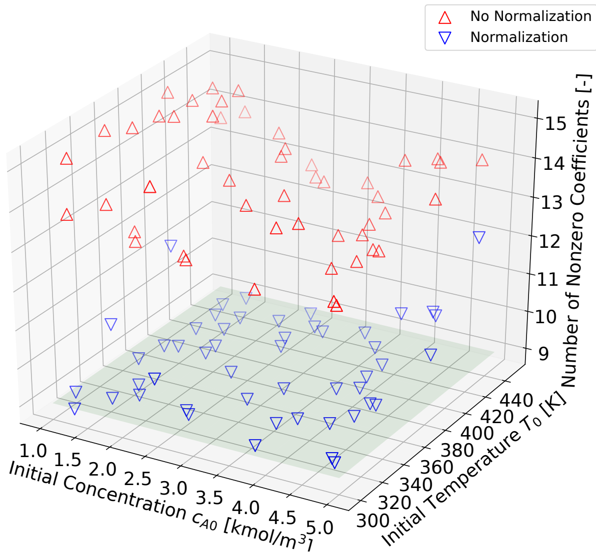

Fig. 2. Number of nonzero coefficients of the 51 identified models as a function of the initial conditions c_{A0}, T_0.

4. CONCLUSION

The effect of normalising the dictionary of candidate functions was evaluated with 51 data sets obtained from varying the initial conditions of the model. It was shown that both process dynamics and controller dynamics can be identified accurately ($R^2 = 1$). The normalisation of the dictionary was shown to be beneficial to promote sparsity. In future work, the proposed framework could be tested with data coming from black-box models, e.g., from the process simulation environment UniSim Design. Also, real process data could be used or additional Gaussian white noise could be added to the input data. In order to determine the performance limit of the proposed framework, local differentiation methods, e.g., the Savitzky-Golay filter, or global differentiation methods, e.g., the total variation derivative, could be evaluated. Furthermore, the framework could be extended to also allow the identification of the differential part of a proportional-integral-differential (PID) controller and other controller structures.

REFERENCES

Brunton, S.L., Proctor, J.L., and Kutz, J.N. (2016). Discovering governing equations from data by sparse identification of nonlinear dynamical systems. *Proceedings of the national academy of sciences*, 113(15), 3932–3937.

Wang, W.X., Yang, R., Lai, Y.C., Kovanis, V., and Grebogi, C. (2011). Predicting catastrophes in nonlinear dynamical systems by compressive sensing. *Physical review letters*, 106(15), 154101.