Systems & Control Transactions

Research Article
Foundations of Computer Aided Process Design (FOCAPD 2024)
Breckenridge, Colorado, USA. July 14-18, 2024
Peer Reviewed Conference Proceeding

Model assessment for Design of Future Manufacturing systems using Digital Twins: A case study on a single-scale pharmaceutical manufacturing unit

Prem Jagadeesan[a] and Shweta Singh [a,b,c*]

a Department of Agricultural and Biological Engineering, Purdue University, West Lafayette, IN, US
b Division of Ecological and Environmental Engineering, Purdue University, West Lafayette, IN, US
c Davidson School of Chemical Engineering (By Courtesy), Purdue University, West Lafayette, IN, US
* Corresponding Author: singh294@purdue.edu.

ABSTRACT

Designing a digital twin will be crucial in developing automation-based future manufacturing systems. The design of digital twins involves data-driven modelling of individual manufacturing units and interactions between the various entities. The goals of future manufacturing units such as zero waste at the plant scale can be formulated as a model-based optimal control problem by identifying the necessary state, control inputs, and manipulated variables. The fundamental assumption of any model-based control scheme is the availability of a "reasonable model", and hence, assessing the goodness of the model in terms of stability and sensitivity around the optimal parameter value becomes imperative. This work analyses the data-driven model of an acetaminophen production plant obtained from SINDy, a nonlinear system identification algorithm using sparse identification techniques. Initially, we linearize the system around optimal parameter values and use local stability analysis to assess the stability of the identified model. Further, we use what is known as a conditional sloppiness analysis to identify the sensitivity of the parameters around the optimal parameter values to non-infinitesimal perturbations. The conditional sloppiness analysis will reveal the geometry of the parameter space around the optimal parameter values. This analysis eventually gives valuable information on the robustness of the predictions to the changes in the parameter values. We also identify sensitive and insensitive parameter direction. Finally, we show using numerical simulations that the linearized SINDy model is not good enough for control system design. The pole-placement controller is not robust, and with high probability, the control system becomes unstable to very minimum parameter uncertainty in the gain matrix.

Keywords: Dynamic Modelling, System Identification, Stability, Sloppiness, Identifiability

INTRODUCTION

Design of future manufacturing systems will benefit from building digital twins that can inform the controller design at plant scale. Several future manufacturing goals such as planning and scheduling for zero waste at the plant scale can be formulated as a control system design problem, where an optimal control problem can be formulated and solved.

The design of optimal control mandates a reasonable model. Developing a mechanistic model at the plant scale might involve hundreds of state variables and parameters; hence we adopt a data-driven nonlinear system identification approach known as SINDy to identify a reduced-order parsimonious model in this work. SINDy uses the idea of sparse identification to discover the underlying governing equations [2]. The SINDy algorithm has already been used to design an entire algal biodiesel industrial network for sustainable design of carbon capture and utilization technologies [3]. In addition to this, SINDy has also been used to identify governing equations of unit operations in a plant and natural systems [7]. In previous work, the authors have used the SINDy algorithm to identify a reduced order dynamical model for the distillation column [6].

The models developed in the above works were satisfactory in replicating the system dynamics; however, the model has to satisfy additional requirements for designing control systems. The critical factors that affect the control system design are stability, model and parameter uncertainty. The seminal work of Bhattacharyya et al [5] showed that while designing robust and optimal controllers such as H_2 and H_∞; a very small parameter uncertainty in the controller parameters will result in an unstable control system. They argue that the fragility of the controller is a result of the parameter sensitivity of the plant that is transferred to the controller. Hence, it becomes imperative to assess the sensitivity of the plant before the controller design; otherwise, uncertainty in the controller output will impact the overall performance metrics.

In this work, we propose a method to analyze the control relevance of the SINDy model; even though this method is applied to models developed from SINDy, in general, this proposed method can be used for any surrogate dynamical model. The novelty in the present work is proposing a new method to assess the robustness of a pole-placement control system design by assessing the model's parameter space by introducing the concept of conditional sloppiness. In general, it is a novel method to assess whether the estimated model is control-relevant. As a first step, we analyze the stability of the linearized model around the operating point. We use sloppiness analysis as a next step to characterize the model's behaviour around the nominal parameter set. Sloppiness is a phenomenon where there are regions in the parameter space over which model predictions are nearly identical. The role of sloppiness in system identification has been extensively studied in the past two decades [1,4]. Here, we use what is known as conditional sloppiness to assess the model sensitivity. Together with stability and sloppiness analysis we provide directions to refine the estimated model. When the model sensitivity index is very high in the vicinity of the parameter space, the model is unsuitable for controller design. This has been demonstrated using a simple pole-placement controller design.

The rest of the paper is organized as follows: Section 2 presents the preliminary concepts, Section 3 illustrates the detailed methodology for assessing the model structure, we assess the goodness of the model of a pharmaceutical node (single plant) in Section 4, and the paper ends with some concluding remarks in Section 5.

PRILIMINARIES

Local Stability Analysis

Analysing the stability of the model plays a crucial role in designing the controllers. The dynamics of industrial systems are predominantly represented by a set of first-order nonlinear differential equations, these are known as state-space models. The set of solution to these nonlinear differential equations are known as state trajectories. A system is completely characterized by the values of the state variables at any given instance of time. The generic nonlinear model representation is given below

$$M: \begin{cases} \frac{dx(t)}{dt} = f(x(t), u(t), \theta) \\ y(t) = g(x(t), u(t), \theta) \end{cases} \quad (1)$$

where, $x(t)$ is the state vector, $u(t)$ is the input vector and θ is the parameter vector. Even though the dynamics is nonlinear, in most cases it can be approximated to a linear dynamics around the operating region. Hence, in this work we use linear stability analysis on the linearized state space model of Eqn 1. The linearized model is given in Eqn 2.

$$\widetilde{M}: \begin{cases} \dot{x} = Ax(t) + Bu(t) \\ y(t) = Cx(t) + Du(t) \end{cases} \quad (2)$$

where A, B, C and D are state-space matrices obtained by evaluating Jacobin of Eq (1) at the operating point (x^*, u^*)The eigenvalues of the A matrix will indicate the stability of the linear perturbation system (2).

Sloppiness

In models with nonlinear predictors, often there are large regions in the parameter space over which the model predictions are nearly identical, this is known as sloppiness or model sloppiness. For infinitesimal perturbations sloppiness is quantified by the inverse of the condition number of the Hessian of the cost-function. The Hessian of the cost function can be approximated as

$$H_{ij} = \frac{1}{N} \sum_{n=1}^{N} \frac{\partial y}{\partial \log \theta_i} \frac{\partial y}{\partial \log \theta_j} \quad (3)$$

where y denotes model output. More formally, for non-infinitesimal perturbations, sloppiness can be conditioned on the experiment space known as conditional sloppiness. A model $\mathcal{M}$ is conditionally (ϵ, δ) sloppy with respect to an experiment space $\mathcal{Z}_{\mathcal{M}}$ at $\theta^* \in \mathcal{I} \subset \mathcal{D}_{\mathcal{M}}$,if

$$||\theta^* - \theta_1||_2 > \delta \ \forall \theta \in \mathcal{S} \subset \mathcal{I} \quad (4)$$

$$||y(\theta^*, t) - y(\theta_1, t)||_2^2 < \epsilon \forall u \in \mathcal{Z} \subset \mathcal{Z}_{\mathcal{M}} \quad (5)$$

for every (θ_1, θ^*) satisfying (4) and (5). ϵ is arbitrarily small . $\delta \gg \epsilon$.

The role of sloppiness in the system identification has been extensively studied in. Sloppiness often affects the uncertainty in the parameter estimates. it is well known the uncertainty in the model structure and parameter estimates affects the robustness of the controller and hence, assessing the parameter uncertainty of the model becomes imperative to a satisfactory control system design. In this work, we use conditional sloppiness analysis to assess the insensitivity in the parameter directions in SINDy models.

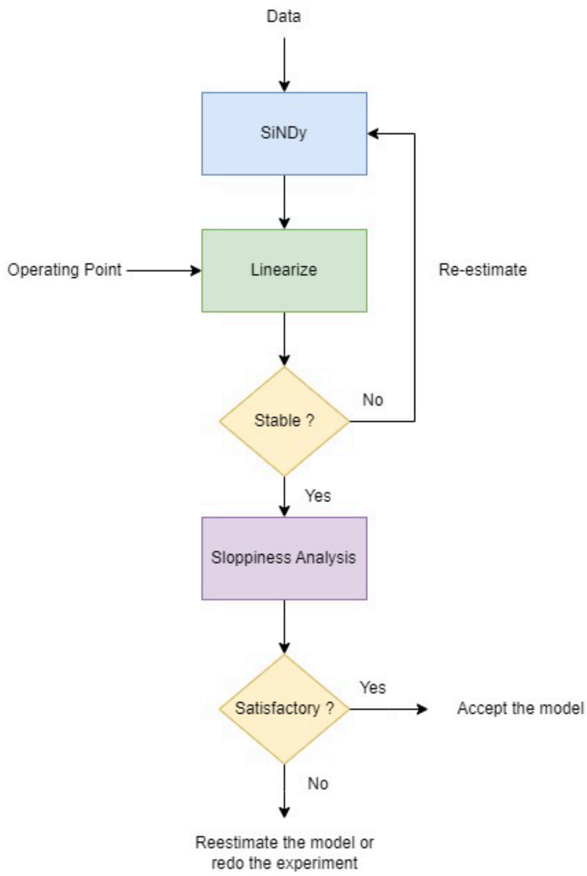

Figure 1: Algorithm for model assessment.

METHODOLOGY

This section illustrates the method proposed for assessing the goodness of the model estimated using the SINDy algorithm. However, the method proposed, in general, can be used to evaluate any model. The proposed method has two significant steps: Firstly, assessing the stability of the local perturbation model (Linearized) and model sloppiness. As a next step, we construct what is known as a $(\delta - \gamma)$ plot as proposed in [1] for conditional sloppiness analysis around the optimal parameter estimated from the SINDy algorithm. The central idea of this analysis is to characterize the model's behaviour around the point of interest in the parameter space; this is done by constructing an n-ball and evaluating the change in the model's output for all the parameters inside the n-ball with respect to the reference point. The procedure for constructing the $(\delta - \gamma)$ plot is in Figure 2.

One of the main advantages of the proposed method is its ability to identify the parameters that are likely to be estimated with poor precision. When those parameters belong to stiff region/sensitive region, then with high probability, the controller system designed may become fragile. In the next section, we demonstrate the working of the proposed method in a dynamical model of an industrial node developed from the SINDy algorithm.

Numerical Results

In this section, we demonstrate the working of the proposed method in a model developed for acetaminophen production plant.

A linearized state-space model of acetaminophen production network

To demonstrate the working of the proposed method, we consider a process where Para-

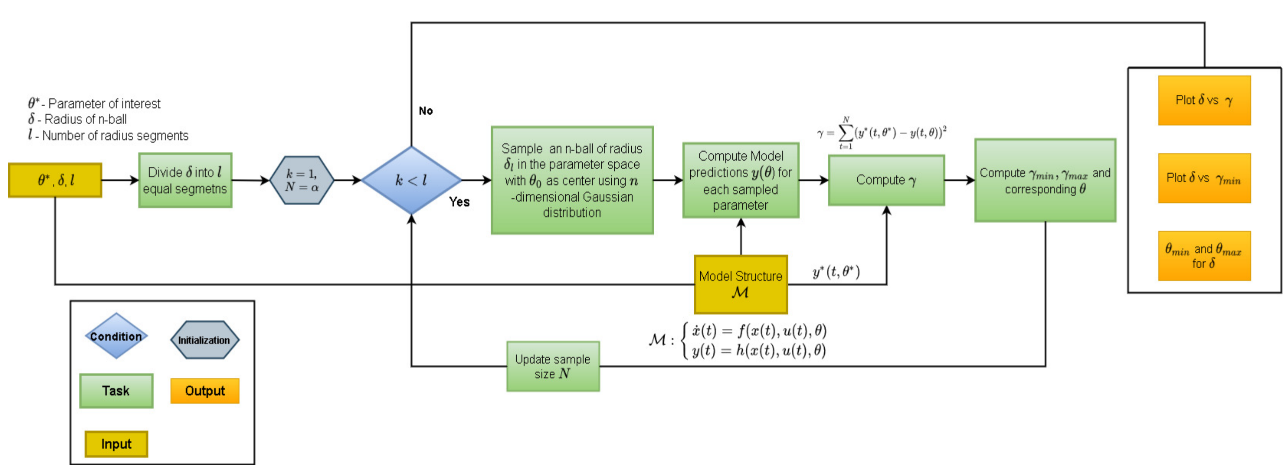

Figure 2: Algorithm to perform conditional sloppiness analysis

Aminophenol(PAP) reacts with Acetic Anhydride to produce Acetaminophen (A-PAP). Equation 7 is the linearized model obtained from the non-linear SINDy model. The detailed state variables and input variables are given in Table 1. The nonlinear ODE model identified using SINDy algorithm is linearized around the operating point. The Operating point and the linearized model is given in the Table 1 and equation 4

$$\dot{x}(t) = \begin{bmatrix} -16.34 & -5.06 & -15.83 & 9.04 \\ 12.22 & -3.41 & 10.72 & 3.43 \\ -0.07 & 7.85 & -1.10 & -5.63 \\ 3.70 & 0.006 & 2.97 & -3.90 \end{bmatrix} x(t) +$$

$$\begin{bmatrix} 11.15 & 3.21 & 4.39 & -7.56 \\ 2.84 & -0.62 & 2.38 & 7.58 \\ 0.76 & 2.78 & -1.91 & -3.52 \\ -0.03 & 4.80 & 4.36 & -0.96 \end{bmatrix} u(t) \qquad (6)$$

$$y(t) = [1 \quad 0 \quad 0 \quad 0]\, x(t) \qquad (7)$$

where $x_1(t)$ is APAP, $x_2(t)$, $x_3(t)$ and $x_4(t)$ are the waste materials produced and $u_1(t)$ is PAP.Fm, $u_2(t)$ is Acetic Anhydride.Fm, $u_3(t)$ is water and $u_4(t)$ is water

The Eigen values of the system matrix A are given below

$$\lambda(A) = [-19.27 \quad -5.28 \quad -0.1 + 3.43i \quad -0.1 - 3.43i]$$

The system has both real and complex poles with negative real parts, which guarantees that the system is capable of damped oscillations. It is also worth noting that the complex poles have real parts that are close to zero value, which says that the system is on the verge of instability. However, the system is in the verge of instability. In the next section we perform conditional sloppiness analysis to study the sensitivity of the system to the parameter perturbations.

Conditional Sloppiness Analysis

In this section, we do the conditional sloppiness analysis for the unforced system, i.e. the input is turned off in the Eq (6) and the x(1) is measured as the output. The model output is generated with the same initial conditions for t=0 to t=10 seconds. In this work, we analyzed the system for $\delta = 10^{-5}$, an infinitesimal distance from its optimal parameter. The visual plots for the model assessment are given below.

From Fig. 3 it is clear that the model is extremely sensitive in the vicinity of the operating initial condition. The system clearly becomes unstable. In addition to that, it is observed that the system is sensitive is almost identical in all the directions. The Model sensitivity index shows that the model is locally unidentifiable, ie there exist several parameter sets in the vicinity that results in an unstable model. In summary, the model identified by SINDy is extremely sensitive to parameter perturbations and a very small perturbation leads to instability. In the next section we demonstrate the role of this insensitivity in the controller design.

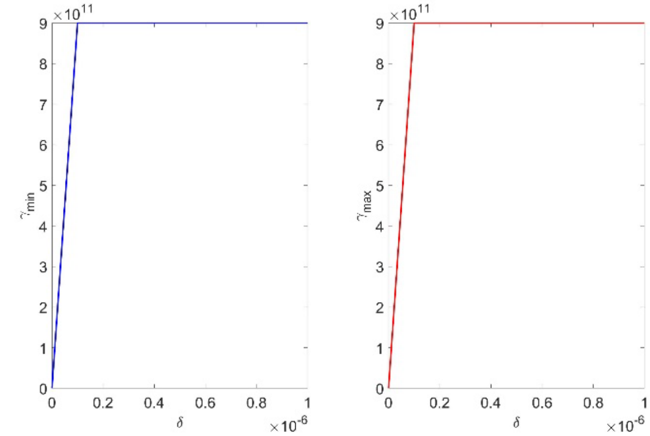

Figure 3: Minimum and Maximum sensitivity plot

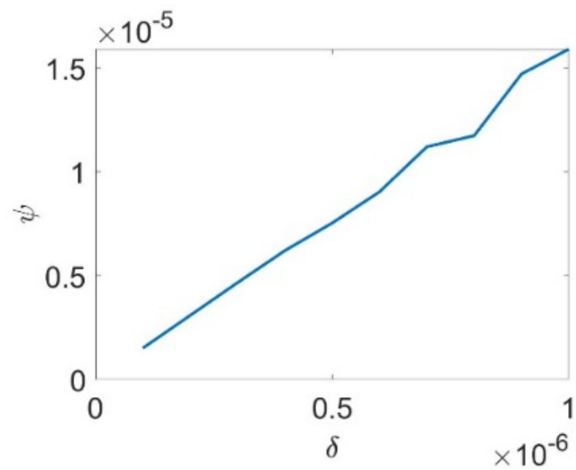

Figure 4: Model sensitivy index

Analysis of controller design

In the previous section, using conditional sloppiness analysis, we showed that the model is very sensitive in the vicinity of the operating region, and an infinitesimal perturbation from the equilibrium position has destabilized the system. In this section, we show that designing the controller for such a system leads to a fragile controller, in the sense a very small perturbation in the controller parameters will destabilize the system. To demonstrate this, we adopt a pole-placement controller design. We place the poles on the following location to stabilize the oscillations in the system p =[-0.5 -1 -1 -0.5].

The gain matrix is obtained for the given A, B and p. The gain matrix is given below. We add a Gaussian random matrix with the controller gain matrix to analyse the controller fragility. We generate a hundred such matrices and compute eigenvalues of the closed-loop system matrix. Ak=A-BK and plot the histogram of the real part of the eigenvalues in Figure 5. It is evident that the controller design is not robust with respect to very small uncertainty in the controller parameters as the distributions shows that are positive real eigen values with significantly hight probability. This analysis shows that the presence of sloppy and stiff directions in the parameter space of the plant affects controller robustness.

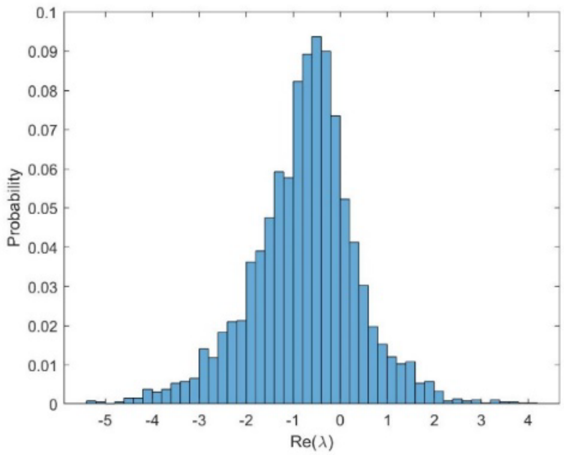

Figure 5: Histogram of real part of the closed loop system matrix.

CONCLUSION

In this work, we proposed a novel method to assess the goodness of data driven surrogate dynamical models developed using the SINDy algorithm for control system design. We analyzed the model generated from the acetaminophen production plant. The original model is a nonlinear ODE. The model is then linearized for the stabilized operating conditions. The analysis revealed that the linearized model is on the verge of instability, and the sloppiness analysis revealed that a tiny perturbation leads to instability. To assess the role of sensitivity in the controller design, we designed a pole placement controller to stabilize the oscillations. We added a small amount of noise to the controller parameters. The Monte Carlo simulations revealed that the closed-loop system would become unstable with a significant probability of minimal uncertainty in the controller parameters. This re-emphasizes that the model identified using the SINDy algorithm is not good enough for control system design. As a logical extension to this work, we propose to formulate and solve a multi-objective robust-optimal control problem to ensure stability, achieve zero waste and maximize the productivity of acetaminophen. This study opens up new avenues in the controller design for sloppy systems.

ACKNOWLEDGEMENTS

The Authors acknowledge Abhimanyu Raj Shekhar for proving the SINDy model for the acetaminophen plant. We are also grateful for the support from the U.S. National Science Foundation CBET FMRG ECO-2229250

REFERENCES

1. Jagadeesan P, Raman K, Tangirala A K (2023) Sloppiness: Fundamental study, new formalism and its application in model assessment. *PLOS ONE* 18(3).
2. Brunton, S. L., Proctor, J. L., & 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. doi:10.1073/pnas.1517384113
3. Shekhar, A. R., Moar, R. R., & Singh, S. (2023). A hybrid mechanistic machine learning approach to model industrial network dynamics for sustainable design of emerging carbon capture and utilization technologies. *Sustainable Energy Fuels*, 7, 5129–5146.
4. Gutenkunst, R. N., Waterfall, J. J., Casey, F. P., Brown, K. S., Myers, C. R., & Sethna, J. P. (10 2007). Universally Sloppy Parameter Sensitivities in Systems Biology Models. *PLOS Computational Biology*, 3(10), 1–8.
5. L. H. Keel and S. P. Bhattacharyya, "Robust, fragile, or optimal?," in *IEEE Transactions on Automatic Control*, vol. 42, no. 8, pp. 1098-1105, Aug. 1997.
6. Farlessyost, W., Singh, S. Reduced order dynamical models for complex dynamics in manufacturing and natural systems using machine learning. *Nonlinear Dyn* 110, 1613–1631 (2022).
7. Subramanian, R., Moar, R. R., & Singh, S. (2021). White-box Machine learning approaches to identify governing equations for overall dynamics of manufacturing systems: A case study on distillation column. *Machine Learning with Applications*, 3, 100014.