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A superstructure-based design of experiments framework for simultaneous domain-restricted model identification and parameter estimation

Calvin Tsay[a], Richard C. Pattison[a], Michael Baldea[a,*], Ben Weinstein[b], Steven J. Hodson[b], Robert D. Johnson[b]

[a] McKetta Department of Chemical Engineering, The University of Texas at Austin, 200 East Dean Keeton St., Stop C0400, Austin, TX 78712, United States
[b] The Procter & Gamble Company, Corporate Function Research and Development, West Chester, OH 45069, United States

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ABSTRACT

We present a novel design of experiments (DOE) approach to incorporate model identification into optimal experimental designs based on a postulated model superstructure and an associated relaxation strategy. We show that an adaptive online design of experiments allows for the accurate estimation of the parameters of a domain-restricted model, as well as the model structure and domain on which that model is valid. We further show that previous attempts at combining model identification and parameter estimation are a special case of this framework (when the objective function is formulated in terms of the trace of the Fisher information matrix), and thus the proposed formulation provides the option to use alternate or more complex objective functions. The efficacy of the proposed framework is shown through two case studies: a batch reactor with Arrhenius-type reactions and a carbon dioxide adsorption system.

1. Introduction

High-fidelity, accurate models are central to process systems engineering and are indispensable for activities such as process design, simulation, and optimization. These models can be built based on physical, chemical, and/or biological laws (first-principles models) or using system identification techniques (empirical models).

The structure of the model and the values of the model parameters are typically determined and verified through an experimental process that has two main goals: (i) *model identification*, i.e., establishing the most appropriate functional form of the model and (ii) *parameter estimation*, i.e., obtaining the values of the model parameters for the chosen functional form. Collecting the data required to build and validate a model can be costly in terms of both resources and time. In addition, resources must be dedicated to testing the model outside of training data range to determine the limits of the model's validity domain. Experimental campaigns must therefore be carefully designed to maximize information gained, while minimizing cost (Franceschini and Macchietto, 2008).

The first attempts at optimizing design of experiments (DOE) were geared towards probing the connection between system inputs (factors) and outputs (responses) (Fisher, 1960). This approach is well suited for constructing "black-box" models, and such techniques typically aim to select the combination of factors to be tested and their values, which maximize information on the input-output relationships. The main class of DOE techniques of this type is factorial methods, which are straight-forward to implement and easily-interpreted; however, factorial designs are not well-suited to handle experiments that are dynamic, in which outputs and inputs are both allowed to vary with time, and/or experiments that contain a large number of input variables. Model-based DOE methods, on the other hand, attempt to exploit knowledge of the underlying mathematical model of the system in establishing the experimental program. Model-based DOE techniques have broad applicability to both static and dynamic models, whether linear or nonlinear and consist of: (i) using model equations to predict the information content of the experiment and (ii) using optimization techniques to determine the experimental conditions that maximize (a measure of) this information content.

In this work, we propose a novel framework for simultaneous model identification and parameter estimation via an adaptive design of experiments. Focusing on constructing models for dynamic systems, we use a model superstructure aggregating a set of dynamic modes that can be selectively activated via a

* Corresponding author.
E-mail address: mbaldea@che.utexas.edu (M. Baldea).

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corresponding set of binary variables. We utilize the superstructure to identify domain-restricted models comprising of a subset of these dynamic modes and the conditions under which the restricted models are valid. We rely on existing methodologies for parameter estimation DOE based on the Fisher information matrix (Asprey and Macchietto, 2000, 2002; Franceschini and Macchietto, 2008), and propose a strategy for online adaptation of the experiments, including varying in time the factors, the corresponding bounds, as well as the bounds on the responses.

The novelty of our contribution consists of:

- A method to include domain-restricted model identification into design of experiments optimization by using a model superstructure and including corresponding relaxed binary variables into the DOE objective function (Section 3.2).
- A framework for an online, adaptive experimental design exploiting the corresponding mixed-integer (MINLP) formulation of the combined model identification/parameter estimation problem (Sections 3.1 and 3.3).
- Incorporating a bisection algorithm during online, adaptive experimental designs to identify the domain on which a domain-restricted model is valid (Section 3.4).

We show that current DOE formulations for simultaneous model identification and parameter estimation that weigh and sum the respective, separate objective functions are a special case of our proposed framework for domain-restricted models. Furthermore, we show the benefits of maximizing the determinant of the information matrix in our new formulation through two case studies: a reaction system with an undesirable side reaction and an adsorption system.

We dedicate this paper to Professor Rafiqul Gani; his work on mixture property estimation for process and product design has been an inspiration in our research and a strong motivation for the model identification and parameter estimation developments in this manuscript.

2. Background

2.1. Class of systems considered

We consider systems that are represented by (systems of) differential and algebraic equations (DAEs), for which the "true" dynamic behavior takes the general form:

$$\begin{aligned} &\mathbf{f}(\dot{\mathbf{x}}(t), \mathbf{x}(t), \mathbf{u}(t), \boldsymbol{\omega}, \boldsymbol{\theta}, t) = 0 \\ &\hat{\mathbf{y}}(t) = \mathbf{h}(\mathbf{x}(t)) \\ &\mathbf{x} \in \mathbf{D}_x, \quad \mathbf{u} \in \mathbf{D}_u \end{aligned} \tag{1}$$

where $\mathbf{x}(t)$ and $\mathbf{u}(t)$ are respectively the vector of state variables and the vector of time-varying controls or input factors, $\boldsymbol{\omega}$ is a vector of constant (time-invariant) controls or inputs, $\boldsymbol{\theta}$ is a vector of model parameters, and $\hat{\mathbf{y}}(t)$ is a vector of measured response variables that are functions of the state variables, $\mathbf{x}(t)$.

Mathematical models of such systems explain and predict systemic behavior based on the input factors and controls within their respective domains, $\mathbf{D}_x$ and $\mathbf{D}_u$. Practically speaking, models are often abridged, excluding and/or replacing some variables present in the true physical system, resulting in the general form:

$$\begin{aligned} &\bar{\mathbf{f}}(\dot{\bar{\mathbf{x}}}(t), \bar{\mathbf{x}}(t), \mathbf{u}(t), \boldsymbol{\omega}, \bar{\boldsymbol{\theta}}, t) = 0 \\ &\hat{\mathbf{y}}(t) = \bar{\mathbf{h}}(\bar{\mathbf{x}}(t)) \\ &\bar{\mathbf{x}} \in \bar{\mathbf{D}}_x, \quad \mathbf{u} \in \mathbf{D}_u \end{aligned} \tag{2}$$

where $\bar{\mathbf{x}}$ is the vector of predicted states, $\bar{\mathbf{f}}$ is the abridged model, and $\bar{\boldsymbol{\theta}}$ is the vector of parameters in the abridged model. Further, the domain of an abridged model may be restricted to a subdomain, which we term a **domain of validity**, of the full input factor and control domains ($\bar{\mathbf{D}}_x^r \subseteq \bar{\mathbf{D}}_x$ and $\mathbf{D}_u^r \subseteq \mathbf{D}_u$). These restrictions may be motivated mathematically, e.g. to allow the use of a simpler model, and/or practically, e.g. to avoid undesirable phenomena during the experimental campaign or during system operation. Restricting the domain allows the modeler to ignore some undesirable or difficult-to-model dynamics; however, such **domain-restricted models** can only make accurate predictions in limited regions of the input and state space.

A domain-restricted model for the general system (1) can similarly be written in a general form:

$$\begin{aligned} &\bar{\mathbf{f}}^r(\dot{\bar{\mathbf{x}}}(t), \bar{\mathbf{x}}(t), \mathbf{u}(t), \boldsymbol{\omega}, \bar{\boldsymbol{\theta}}, t) = 0 \\ &\hat{\mathbf{y}}(t) = \bar{\mathbf{h}}(\bar{\mathbf{x}}(t)) \\ &\bar{\mathbf{x}} \in \bar{\mathbf{D}}_x^r, \quad \mathbf{u} \in \mathbf{D}_u^r \\ &\bar{\mathbf{D}}_x^r \subseteq \bar{\mathbf{D}}_x, \quad \mathbf{D}_u^r \subseteq \mathbf{D}_u \end{aligned} \tag{3}$$

where the predicted state variables $\bar{\mathbf{x}}(t)$ and input factors $\mathbf{u}(t)$ are constrained to a subset ($\mathbf{D}^r = \bar{\mathbf{D}}_x^r \times \mathbf{D}_u^r$ - the **domain of validity**) of the full domain $\mathbf{D} = \bar{\mathbf{D}}_x \times \mathbf{D}_u$. The function $\bar{\mathbf{f}}^r$ may be a further abridged or simplified version of the unrestricted model $\bar{\mathbf{f}}$ that excludes dynamic modes present in $\mathbf{D}$ but irrelevant in $\mathbf{D}^r$. More specifically, the unrestricted model $\bar{\mathbf{f}}$ can be thought of as capturing systemic behavior through a set of component functions, or **dynamic modes**, while the restricted model $\bar{\mathbf{f}}^r$ is a set (often a subset) of dynamic modes that can be used to make accurate predictions of the system behavior in a smaller, restricted domain $\mathbf{D}^r \subset \mathbf{D}$.

Simple Example

As an illustrative example, we consider approximating a nonlinear, input-affine model $\dot{x} = \alpha(x) + \beta(x)u$ with a linear model $\dot{x} = ax + bu$. Specifically, we assume a physical process f that is accurately modeled by a nonlinear first-order function $\bar{f}$ with initial condition $x(0) = 0$ and steady-state gain $\bar{\theta}_3$ described by:

$$\alpha(x) = \frac{-x}{\bar{\theta}_1 x^2 + \bar{\theta}_2}, \quad \beta(x) = \frac{\bar{\theta}_3}{\bar{\theta}_1 x^2 + \bar{\theta}_2} \tag{4}$$

which fits in the general DAE form (1), with:

$$\bar{f} = \dot{x} + \frac{x}{g(x)} - \frac{\bar{\theta}_3}{g(x)}u = 0 \tag{5}$$

$$g(x) = \bar{\theta}_1 x^2 + \bar{\theta}_2$$

where the state variable x and input variable u are in domains $D_x = D_u = [0, \infty)$. To reduce mathematical complexity, we can choose to approximate the system with an abridged linear first-order mathematical model of the form:

$$a = \frac{-1}{\bar{\theta}_1^r}, \quad b = \frac{\bar{\theta}_2^r}{\bar{\theta}_1^r} \tag{6}$$

$$\bar{f}^r = \dot{x} + \frac{x}{\bar{\theta}_1^r} - \frac{\bar{\theta}_2^r u}{\bar{\theta}_1^r} = 0$$

While the linear model $\bar{f}^r$ does not fully capture the dynamics of the nonlinear model $\bar{f}$, it can conceivably make accurate predictions over a limited range of the state and input variables x and u. The goal is then to find parameter values $\bar{\theta}_1^r$ and $\bar{\theta}_2^r$ and the domain over which $\bar{f}^r$ can be used to model $\bar{f}$ accurately. We assume the system is modeled accurately with the parameter values $\bar{\theta}_1 = 0.1$, $\bar{\theta}_2 = 2$, and $\bar{\theta}_3 = 1$. Intuitively, we can see that the linear approximation

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