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Optimal input design for model discrimination using Pontryagin's maximum principle: Application to kinetic model structures ☆

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ABSTRACT

The paper presents a methodology for an optimal input design for model discrimination. To allow analytical solutions, the method, using Pontryagin's maximum principle, is developed for non-linear single-state systems that are affine in their joint input. The method is demonstrated on a fed-batch reactor case study with first-order and Monod kinetics.

1. Introduction

Before attempting to estimate the parameters of a given model, one may have to choose the proper model structure among a set of candidates, which may correspond, for instance, to competing scientific hypotheses about the description of some phenomenon (see, e.g., some of the practical examples in Keesman (2011)). The procedure of choosing between model structures is called *model discrimination*. For it to be possible on the basis of (future) experimental data, these models must be *distinguishable*. The distinguishability property can be tested by techniques similar to those used to test models for identifiability (although identifiability of two structures is neither necessary nor sufficient for their distinguishability); see Walter, Lecourtier, and Happel (1984). In practice, of course, the ability to discriminate distinguishable model structures depends on the informational content of the data collected. Optimal experiment design for model discrimination has received some attention in the statistical literature (see, e.g., Atkinson & Cox, 1974; Box & Hill, 1967; Dette & Titoff, 2009), although less than optimal experiment design for parameter estimation did. Applications of experiment design for discrimination can be found in domains as diverse as chemistry Schwaab et al. (2006), machine learning Rajamoney (1993), system biology Kreutz and Timmer (2009), Skanda and Lebiedz (2010) and psychology Myung and Pitt (2009).

For optimal design to be possible, some performance index is needed. *T-optimal design*, as in Atkinson and Fedorov (1975), aims at maximizing some measure of the lack of fit between the output of some model assumed to be true and that of an alternative structure. Ponce de Leon and Atkinson (1991) extend T-optimality to the case where prior probabilities are specified for each of the models to be true, as well as prior distributions for the parameters of these models. *KL-optimal design*, see Lopez-Fidalgo, Tommasi, and Trandafir (2007) and Skanda and Lebiedz (2010), based on the Kullback–Leibler divergence, can be seen as a generalization of T-optimal design of interest under non-normal assumptions. *D_s-optimal design*, as in Studden (1980), applies to the discrimination between two structures with a common part, by attempting to maximize some measure of the precision with which structure-specific parameters are estimated. For an extension to more than two rival structures, see Atkinson and Cox (1974). *Entropy-based design*, as in Box and Hill (1967) and Reilly (1970), assumes that each of the competing structures is given a prior probability and updates the probabilities of the structures after each measurement. The new experiment is then designed to maximize some measure of the decrease in Shannon's entropy to be expected from the next measurement (entropy is minimal when a single model structure has gained all the probability mass).

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Although the proposed method, based on Pontryagin's maximum principle (PMP), may seem to be rather limited at first sight, we think it is nevertheless valuable to study closed form analytical solutions, as these solutions provide direct insight in terms of possible singularities, steady states, parameter sensitivities, etc. We demonstrate the method in a case study using kinetic model structures. Typically, in bio-reactor modeling, a specific kinetic model structure will appear in different equations, as in e.g. oxygen, substrate and biomass balances. In each of the balances the kinetic model will only be corrected by a so-called yield coefficient, expressing the stoichiometric relationship between the components (see e.g. Bastin & Dochain, 1990). Also, in basic physical modeling with its mass balances in the PDE form, we distinguish storage and transport terms from the reaction term. Under the assumption that the reaction term does not depend on the other terms, we can investigate all kinds of kinetic models separately. Thus, instead of discriminating potential multi-state models for the whole reactor system, we can focus on a single-state system that only contains the kinetic model.

2. Preliminaries

In the paper, as already motivated in the previous paragraph, and for the purpose of introducing the idea of optimal input design for model discrimination using analytical solutions, we limit ourselves to the case of two non-linear scalar state equations that are affine in their joint input. Hence, without explicitly referring to the parameter vectors to simplify notation, two competitive model structures are defined by the following state equations

$$\dot{x_1}(t) = f_1(x_1(t)) + b_1 u(t) \tag{1}$$
$$\dot{x_2}(t) = f_2(x_2(t)) + b_2 u(t) \tag{2}$$

with $x_1(t)$ and $x_2(t)$ being scalar states, $u(t)$ the joint control input, and $f_1(\cdot),\ f_2(\cdot)$ non-linear functions. In what follows, it is assumed that $f_1(x_1(t)), f_2(x_2(t)) \in \mathcal{R}^2[(-\infty, \infty)]$. For the readability of the solutions only, it is further assumed that the states are directly observed so that $y_i(t) = x_i(t)$ for $i = 1, 2$. Hence, it suffices to derive a control law in terms of $x_i(t)$. Since our aim is to optimally discriminate between models from *new* experiments, it is intuitively appealing to focus on the norm of the difference of the predicted output signals. Here, our concern is to find a control law that optimally discriminates between competitive, single-input—single-state models. A similar approach to the OID problem, but then for parameter estimation using PMP, is presented by Keesman and Stigter (2002) and Stigter and Keesman (2004).

3. Optimal input design

3.1. Singular control using squared 2-norm of the differences and linear input costs

Let us start from the general system description given in (1)–(2). As a measure of optimality, the following utility function, which includes the linear costs of the control input, is introduced:

$$J = \int_{t=0}^{t_f} (x_1(\tau) - x_2(\tau))^2 - \rho u(\tau) d\tau \tag{3}$$

under the dynamic constraints given by (1)–(2) and the (practical) input constraints:

$$u_{\min} \le u(t) \le u_{\max}, \quad \forall t \ge 0 \tag{4}$$

with, in what follows, $u_{\min} = 0$ and $u_{\max}$ being the maximum allowed value, frequently determined by the equipment. Consequently, the OID problem leads to a constrained optimization problem, where our goal is to maximize (3).

For finding analytical solutions to the problem, define the Hamiltonian

$$\mathcal{H}(x(t), \lambda(t)) \triangleq -(x_1(t) - x_2(t))^2 + \rho u(t) + \sum_{i=1}^{2} \lambda_i(t)\dot{x}_i(t) \tag{5}$$

where $\lambda_i(t),\ i = 1, 2$, are the co-states. The last term on the right-hand side of (5) is included to fulfil the dynamic constraints, given by (1)–(2) (see e.g. Stengel (1994) for details). Let $\mathcal{U}$ be the admissible set of input trajectories defined by (4). Pontryagin's maximum principle states that the input $u(t) \in \mathcal{U}$ that minimizes $\mathcal{H}$ is optimal and thus in this case maximizes J.

The following holds (see, e.g., Bryson, 1999):

$$\dot{\lambda}_1(t) = -\frac{\partial \mathcal{H}}{\partial x_1} = 2x_1(t) - 2x_2(t) - \dot{f}_1\lambda_1(t) \tag{6}$$
$$\dot{\lambda}_2(t) = -\frac{\partial \mathcal{H}}{\partial x_2} = -2x_1(t) + 2x_2(t) - \dot{f}_2\lambda_2(t) \tag{7}$$

where, for simplicity of notation, $f_i(x_i(t))$ and its derivatives $\frac{df_i(x_i)}{dx_i}$ are denoted as $f_i, \dot{f}_i$, *etc.*

Since $\mathcal{H}$ does not explicitly depend on time, a first integral of the problem is $\mathcal{H} = c$ with c being a real constant. Also, since the final time t_f is assumed to be unknown and no terminal conditions are specified (determining the value of the co-states at t_f), this constant can be assumed equal to zero. Furthermore, since the problem is affine in the bounded control variable $u(t)$ (4), three types of constraints on the optimal control can be found

$$\begin{aligned} &u(t) = u_{\max} \quad \text{if } s_f < 0 \\ &0 \le u(t) \le u_{\max} \quad \text{if } s_f = 0 \\ &u(t) = 0 \quad \text{if } s_f > 0 \end{aligned} \tag{8}$$

where $s_f = \partial\mathcal{H}/\partial u$ is the so-called *switching function*. The case $s_f = 0$ corresponds to a singular arc. A singular controller that minimizes the Hamiltonian $\mathcal{H}$ over all possible input sequences $u(t)$ can be derived by setting

$$\forall i \in \{0, 1, 2, \ldots\}: \quad \frac{d^i}{dt^i}\frac{\partial \mathcal{H}}{\partial u} = 0. \tag{9}$$

Hence, the singular control law is derived by solving a set of algebraic equations, generated through repeated differentiation of the Pontryagin optimality condition $\frac{\partial \mathcal{H}}{\partial u} \equiv 0$ on the compact interval $[t_1, t_2]$. In order to determine the optimal input $u(t)$ in (1)–(2) explicitly two differentiations are needed, presuming that u appears in one of the equations of (9). For $i = 0$, and thus for $\partial\mathcal{H}/\partial u = s_f = 0$, we get $s_f = \rho + b_1\lambda_1(t) + b_2\lambda_2(t) = 0$. Hence, $\lambda_1(t) = -\frac{\rho + b_2\lambda_2(t)}{b_1}$, and the condition $\mathcal{H} \equiv 0$ gives $\lambda_2(t) = (\rho f_1 + b_1(x_1 - x_2)^2)/(-b_2 f_1 + b_1 f_2)$. Subsequent differentiation of the condition $\frac{\partial \mathcal{H}}{\partial u} = 0$, assuming that the condition holds on an interval, yields for $i = 1$ and using (6)–(7) the so-called *singularity condition*:

$$\begin{aligned} \phi(t) = {} & [b_1(f_2(2(b_1 - b_2)x_1 - 2(b_1 - b_2)x_2 + \rho\dot{f}_1) \\ & + b2(x_1 - x_2)^2(\dot{f}_1 - \dot{f}_2)) - b_2 f_1(2(b_1 - b_2)x_1 \\ & - 2(b_1 - b_2)x_2 + \rho\dot{f}_2)]/[-b_2 f_1 + b_1 f_2] = 0 \end{aligned} \tag{10}$$

with $-b_2 f_1 + b_1 f_2 \neq 0$. The corresponding singular control law, found from (9) for $i = 2$, is given by

$$\begin{aligned} u^*(t) = {} & \Big(2b_2(-b_1 + b_2)f_1^2\dot{f}_2 - b_1\dot{f}_1(2(b_1 - b_2)f_2^2 \\ & + b_2(x_1 - x_2)^2(\dot{f}_1 - \dot{f}_2)\dot{f}_2 + b_2 f_2(x_1 - x_2) \\ & * (2\dot{f}_1 - 2\dot{f}_2 + (x_1 - x_2)\ddot{f}_2)) + f_1(b_1 b_2(x_1 - x_2) \\ & * \dot{f}_2(2\dot{f}_1 - 2\dot{f}_2 + (x_1 - x_2)\ddot{f}_1) + 2(b_1 - b_2) \end{aligned}$$