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Brief paper

An economic objective for the optimal experiment design of nonlinear dynamic processes[☆]

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ABSTRACT

State-of-the-art formulations of optimal experiment design problems are typically based on a design criterion which allows us to optimize a scalar map of the predicted variance–covariance matrix of the parameter estimate. Famous examples for such scalar objectives are the A-criterion, the E-criterion, or the D-criterion, which aim at minimizing the trace, maximum eigenvalue, or determinant of the variance–covariance matrix. In this paper, we propose a different way of deriving an *economic* design criterion for the optimal experiment design. Here, the corresponding analysis is based on the assumption that our ultimate goal is to solve an optimization problem with a given economic objective that depends on uncertain parameters, which have to be estimated by the experiment. We illustrate the approach by studying a fedbatch bioreactor.

1. Introduction

Nonlinear differential equation models are nowadays indispensable tools for the analysis, design, operation and optimization of dynamic processes. For an accurate modeling, it is necessary to collect experimental data by performing experiments. To limit this experimental burden *optimal experiment design* (OED) methods have been developed. The idea is to design experiments which reveal the highest amount of information. The field of OED (for parameter estimation) has been founded by Fisher (1935) and has been extended to static linear and nonlinear models in Box and Lucas (1959) and Kiefer and Wolfowitz (1959). The transition to dynamic systems has been accomplished in Gevers and Ljung (1986) and Mehra (1974) for the linear and in Espie and Machietto (1989) for the nonlinear case. For a more detailed overview, the reader is referred to Franceschini and Macchietto (2008) and Pukelsheim (1993). With respect to numerical implementations, state-of-the-art methods are described in Balsa-Canto, Alonso, and Banga (2010), Hoang, Barz, Merchan, Biegler, and Arellano-Garcia (2013), Körkel, Kostina, Bock, and Schlöder (2004), Schenkendorf, Kremling, and Mangold (2009) and Telen et al. (2013). In practice, model-based process optimization is meant to improve the performance of the process without spending (too) much effort on performing experiments.

This paper follows the philosophy to design experiments with respect to the intended model application, a well-established concept for linear systems (Gevers & Ljung, 1986), in particular, in the context of joint design for control and identification (Gevers, 1993; Hjalmarsson, 2005). However, in OED for nonlinear dynamic processes these concepts are less established, and thus we propose in this paper a way to formulate a design criterion that leads to a new concept named the *economic optimal experiment design* for nonlinear dynamic systems. We assume that our ultimate goal is to solve an optimal control problem with economic objective that depends on an unknown parameter vector p. If we solve this optimal control problem based on an estimate of the parameters p

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in place of their unknown exact values, we will find a sub-optimal control input. Now, the aim of economic OED is to reduce the expected optimality gap that is associated with solving the optimal control problem based on an estimate for p. The contribution is that we formulate and approximately solve such economic OED problems, yielding an optimally weighted A-criterion that is invariant under affine parameter transformations.

We start in Section 2 with a motivating example and briefly review the idea of OED in Section 3. Our contribution is presented in Sections 4 and 5, where we discuss how to formulate economic OED problems. Section 6 presents a case study and Section 7 the conclusions.

2. A motivating example

We consider a dynamic model for a continuously stirred tank reactor (CSTR) in which a *Van de Vusse* reaction takes place (Bonilla, Diehl, Logist, De Moor, & Van Impe, 2010): $A \overset{k_1}{\to} B \overset{k_2}{\to} C$ and $2A \overset{k_3}{\to} D$. Since the substances C and D are unwanted and do not react further, our dynamic model is given by

$$\dot{c}_A = \frac{\dot{V}}{V_R}(c_{A0} - c_A) - k_1 c_A - k_3 c_A^2 \tag{1}$$

$$\dot{c}_B = -\frac{\dot{V}}{V_R} c_B + k_1 c_A - k_2 c_B, \tag{2}$$

where c_A and c_B are the concentrations of the substances A and B. The feed inflow has a known concentration $c_{A0} = 5.1\ \frac{\mathrm{mol}}{\mathrm{L}}$ and its flow rate $\dot{V}$ can be controlled. The reactor capacity $V_R = 10$ L is given, but the reaction rates $k_1 = k_2$ and k_3 are unknown, i.e., we have two free uncertain parameters. For simplicity of presentation, we assume in this section that we want to operate the CSTR at the steady state optimizing the product concentration c_B:

$$\max_{c_A, c_B, \dot{V}} \ c_B \quad \text{s.t.} \begin{cases} 0 = \dfrac{\dot{V}}{V_R}(c_{A0} - c_A) - k_1 c_A - k_3 c_A^2 \\ 0 = -\dfrac{\dot{V}}{V_R} c_B + k_1 c_A - k_1 c_B. \end{cases}$$

The above expression for c_B can be maximized explicitly finding that the optimal flow rate is given by[2] $\dot{V}^* = k_1 V_R$. This explicit expression for the optimal flow rate $\dot{V}^*$ reveals that the optimal input depends on the unknown parameter k_1 only, while the accuracy of our estimates for the other unknown parameter k_3 is completely irrelevant for maximizing the steady state product concentration c_B. What would we have done if we had not have found this explicit expression for $\dot{V}^*$? Clearly, if we do not employ analysis tools for getting an insight about the parametric dependences of a process, we might spend a lot of effort or money for measuring irrelevant parameters, in this example k_3, as we might not realize in advance that the values of these parameters are irrelevant for computing an optimal operation point. Thus, for a more involved process, we need advanced numerical tools to analyze which parameter values are more relevant than others in order to design an optimal experiment. The aim of this paper is to develop such numerical tools.

3. Optimal experiment design

We are interested in a maximum likelihood parameter estimation problem of the form

$$\min_{x,p} \frac{1}{2} \|M(x,p) - \eta\|_{\Sigma^{-1}}^2 + \frac{1}{2} \left\|p - \hat{p}\right\|_{\Sigma_0^{-1}}^2 \quad \text{s.t. } G(x,u,p) = 0. \tag{3}$$

Here, $p \in \mathbb{R}^{n_p}$ is the parameter which we want to estimate, $u \in \mathbb{R}^{n_z}$ is a given control input which can be adjusted for taking the measurements, and $\eta \in \mathbb{R}^{n_M}$ is the measurement value. The measurement function M and the right-hand side function G are assumed to be continuously differentiable. The function G can for example denote a steady state equation, where x would denote a single steady state, but it could also arise from discretizing a dynamic system (Bock & Plitt, 1984). Finally, $\Sigma \in \mathbb{S}_+^{n_M}$ and $\Sigma_0 \in \mathbb{S}_+^{n_p}$ denote the variance–covariance matrix of the measurement error and the given initial parameter estimate $\hat{p}$, respectively.

The optimal experiment design aims at minimizing a suitable scalar design criterion $\Phi : \mathbb{S}_+^{n_p} \to \mathbb{R}$ of the approximate variance–covariance matrix $V(u,\hat{p}) := \mathcal{F}(u,\hat{p})^{-1}$ assuming that the Fisher information matrix, given by

$$\mathcal{F}(u,\hat{p}) := \Sigma_0^{-1} + M_p(x_s(u,\hat{p}),u,\hat{p})^\mathsf{T} \Sigma^{-1} M_p(x_s(u,\hat{p}),u,\hat{p}),$$

is invertible. Here, $\hat{p} \in \mathbb{R}^{n_p}$ is the currently best available estimate for the parameter, $x_s(u,\hat{p})$ denotes the solution of the implicit state equation

$$G(x_s(u,\hat{p}),u,\hat{p}) = 0,$$

which is assumed to be unique, and

$$M_p(x_s(u,\hat{p}),u,\hat{p}) := -\frac{\partial M}{\partial x}\left(\frac{\partial G}{\partial x}\right)^{-1}\frac{\partial G}{\partial p} + \frac{\partial M}{\partial p}\Bigg|_{(x_s(u,\hat{p}),u,\hat{p})}.$$

In this context, the Jacobian matrix, given by

$$\frac{\partial G(x_s(u,\hat{p}),u,\hat{p})}{\partial x},$$

can be assumed to be invertible for all feasible inputs u such that the above expression for M_p is well-defined. The optimal experiment design problem of our interest can now be written as

$$\min_u \ \Phi\left(V(u,\hat{p})\right) \quad \text{s.t. } H(u) \leq 0.$$

Here, H is a given constraint function.

4. Second order expansion of optimality loss

Our ultimate goal is to solve the "economic" optimization problem

$$\min_{x,u} \ F(x,u,p_{\text{real}}) \quad \text{s.t.} \begin{cases} G(x,u,p_{\text{real}}) = 0 \\ H(u) \leq 0, \end{cases} \tag{4}$$

which depends on an unknown parameter $p_{\text{real}} \in \mathbb{R}^{n_p}$. The functions F, G, and H are assumed to be twice continuously differentiable and the state $x_s(u,p_{\text{real}})$ of the real dynamic process is for any given u assumed to be determined uniquely by the equation

$$G(x_s(u,p_{\text{real}}),u,p_{\text{real}}) = 0.$$

Similar to the non-degeneracy condition from the previous section, the matrix

$$\frac{\partial G(x_s(u,p_{\text{real}}),u,p_{\text{real}})}{\partial x}$$

is assumed to be invertible for all feasible inputs u. Since p_{real} is unknown, a reasonable practical strategy is to first design an experiment and to collect measurements in order to compute an estimate

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[2] In order to derive the expression for the optimal flow rate, it is helpful to employ the explicit relation

$$c_B = -\frac{k_1}{2k_3} + \sqrt{\left(\frac{k_1}{2k_3}\right)^2 + \frac{k_1^2 c_{A0} V_R \dot{V}}{k_3(k_1 V_R + \dot{V})^2}}.$$