Computers and Chemical Engineering 94 (2016) 212–220

Contents lists available at ScienceDirect

Computers and Chemical Engineering

journal homepage: www.elsevier.com/locate/compchemeng

Multi-purpose economic optimal experiment design applied to model based optimal control

D. Telen[a], B. Houska[b], F. Logist[a], J. Van Impe[a,*]

[a] KU Leuven, Chemical Engineering Department, BioTeC+ & OPTEC, Gebroeders De Smetstraat 1, 9000 Gent, Belgium
[b] ShanghaiTech University, School of Information Science and Technology, 319 Yueyang Road, Shanghai 200031, China

ARTICLE INFO

Article history:
Received 28 August 2015
Received in revised form 4 May 2016
Accepted 3 July 2016
Available online 3 August 2016

Keywords:
Optimal experiment design
Optimality loss
Multi-purpose design
Optimal control
Variance–covariance matrix

ABSTRACT

In contrast to classical experiment design methods, often based on alphabetic criteria, economic optimal experiment design assumes that our ultimate goal is to solve an optimization or optimal control problem. As the system parameters of physical models are in practice always estimated from measurements, they cannot be assumed to be exact. Thus, if we solve the model based optimization problem using the estimated, non-exact parameters, an inevitable loss of optimality is faced. The aim of economic optimal experiment design is precisely to plan an experiment in such a way that the expected loss of optimality in the optimization is minimized. This paper analyzes the question how to design economic experiments under the assumption that we have more than one candidate objective function. Here, we want to take measurements and estimate the parameters before we actually decide which objective we want to minimize.

1. Introduction

Model-based optimization is a mathematical tool that has applications in almost all fields of engineering. However, whenever model-based optimization is used to simulate or control real-world processes, an application of computer based numerical methods has to be preceded by experiments that allow us to identify a suitable model and to estimate its associated parameters. Optimal experiment design methods, as originally invented by Fisher (1935), are sought to employ optimization methods already before or during an actual experiment is performed in order to design the experiment in such a way that its expected information content is maximized.

Historically, optimal experiment design (OED) methods have been developed by many authors, for regression models one of the earliest works is Kiefer and Wolfowitz (1959) while the field for nonlinear dynamic systems started with Espie and Macchietto (1989). For a recent discussion on the state-of-the-art the reader is referred to Franceschini and Macchietto (2008) for an overview. The question how to formulate the objective of OED mathematically has no universal answer and from this perspective it is not surprising that many suggestions have been made in the literature. Existing approaches are usually based on minimizing a "*suitable*" scalar measure of the inverse of the Fisher information matrix (or a direct approximation of the parameter variance–covariance matrix (Heine et al., 2008)) such as the trace, determinant, maximum eigenvalue, or maximum diagonal element leading to the so-called A-, D-, E-, or M-criterion, which also have statistical interpretations (Franceschini and Macchietto, 2008). Here, an empirical observation (see, e.g., Telen et al., 2012) is that for models with low complexity and a few parameters only, it is—at least from a practical perspective—not excessively important which of the above mentioned objectives is chosen as they often lead to very similar inputs. This empirical observation might also be expected intuitively, since all these design criteria aim at maximizing the "*information content*" of the experiment in one or the other sense.

However, once we consider more complex models with a moderate to large amount of unknown parameters, different OED objectives may lead to significantly different experiments and, in this case, the construction of the OED objective does itself become a modeling problem. In this context, it is important to be aware of the fact that many famous experiment design criteria such as the A- and E-criterion are not even invariant under affine transformations of the parameters (Franceschini and Macchietto, 2008). Consequently, it might not even be clear how to choose a proper scaling of the objective. One way to deal with this issue is to solve a multi-objective OED problem, where a large number of OED problems with different candidate objectives is solved. In this case, the

* Corresponding author.
E-mail address: jan.vanimpe@kuleuven.be (J. Van Impe).

http://dx.doi.org/10.1016/j.compchemeng.2016.07.004
0098-1354/

decision which of the corresponding experiments will be implemented, is left to a human decision-maker (Logist et al., 2012; Telen et al., 2012). It is clear that such a multi-objective approach is an effective solution for problems, where it is enough to take a small amount of candidate objectives into account. However, as soon as we start screening a 3-, 4- or even higher dimensional Pareto front, the multi-objective approach is limited by the curse of dimensionality.

This paper is about how we can construct suitable objectives for optimal experiment design under the assumption that our ultimate goal is to solve model-based optimization or optimal control problems based on the parameters that are found from the experiment. In this context, it is interesting to mention that for linear systems it is a well-established concept to design experiments with respect to the intended model application (Gevers and Ljung, 1986). This concept has also been elaborated in the context of joint design for control and identification (Hjalmarsson, 2009; Larsson et al., 2015). In Hjalmarsson (2009) this idea has been elaborated and generalized for a broad application spectrum by introducing a generic concept considering quadratic performance degradation costs that can be used to quantify the goal of the experiment design, while in Larsson et al. (2015) the methodology is applied to an industrial case study. Moreover, in Recker et al. (2012) the intended use of the model is taken heuristically into account for the first time for formulating the objectives in nonlinear model-based optimization and optimal experiment design problems. The problem formulation proposed in Houska et al. (2015) leads to a recent concept named "*Economic Optimal Experiment Design*", which is reviewed in Section 2. The main contribution of this paper is that we extend the idea of economic optimal experiment design for the case that we have more than one application in mind in Section 3. In other words, we want to design experiments that allow us to estimate parameters before we choose an objective function that we want to minimize based on the estimated parameters. Here, our assumption is that we have a set of candidate model applications, i.e., objective functions, in mind when we design the experiment. This can be a typical problem in large reaction networks or plant wide dynamic models. Focusing on the production of some specific desired products (or different cell growth aims), will require an accurate estimation of the (kinetic) parameters in the corresponding reaction paths/sub units. This can lead to correlated requirements if the reaction paths/sub units are similar or overlapping. If these are hardly overlapping, a correlation between the different economic objectives will not be expected. The corresponding mathematical problem formulation leads to a non-convex min-max optimization problem, which can be reformulated in the form of an equivalent standard nonlinear programming problem, as discussed in Theorem 3.1 of this paper. Section 4 introduces the two illustrative case studies, namely, the Droop model and the Lee–Ramirez bioreactor model of increasing complexity. The numerical results of the case study are described in Section 5. Section 6 concludes the paper.

Notation.

Besides mathematical standard notation, we denote with $\mathbb{S}^n_{++}$ the set of symmetric positive definite matrices. Additionally, we write $A \preceq B$ for two symmetric matrices A and B if the matrix $B - A$ is positive semi-definite. The notation $A^\dagger$ denotes the Moore–Penrose pseudo-inverse of the matrix A.

2. Economic optimal experiment design

In this section, we review the main idea of *economic optimal experiment design* by briefly summarizing some of the basic concepts that have originally been proposed in Houska et al. (2015). For this aim, we start with the most simple case that we are interested in an unconstrained least-squares parameter estimation problem of the form:

$$\min_p \frac{1}{2}\left\|H(u,p)-\eta\right\|^2_{\Sigma^{-1}} + \frac{1}{2}\left\|p-\hat{p}\right\|^2_{\Sigma_0^{-1}}. \tag{1}$$

Here, $H : \mathbb{R}^{n_u} \times \mathbb{R}^{n_p} \to \mathbb{R}^m$ denotes a given measurement function and $\Sigma \in \mathbb{S}^m_{++}$ the variance–covariance matrix of the measurement error. Additionally, an initial parameter estimate $\hat{p} \in \mathbb{R}^{n_p}$ is taken into account, whose precision is assumed to be given in the form of the variance–covariance matrix $\Sigma_0 \in \mathbb{S}^{n_p}_{++}$.

The aim of optimal experiment design is to find an optimal input $u \in \mathbb{R}^{n_u}$, which maximizes the information content of an experiment. Here, information is often quantified in terms of the so-called Fisher information matrix:

$$\mathcal{F}(u,p) := \Sigma_0^{-1} + \left(\frac{\partial H(u,p)}{\partial p}\right)^T \Sigma^{-1} \frac{\partial H(u,p)}{\partial p},$$

whose inverse $V(u,p) := \mathcal{F}(u,p)^{-1}$ can be interpreted as an affine approximation of the variance–covariance matrix of the predicted parameter estimate (Ljung, 1999; Pukelsheim, 1993). The standard identification procedure based optimal experiment design consists of the following steps:

(1) Choose a scalar experiment design criterion $\Phi : \mathbb{S}^{n_p}_{++} \to \mathbb{R}$ and solve the input design problem:

$$u^* \in \operatorname*{argmin}_u \Phi\left(V(u,\hat{p})\right) \quad \text{subject to} \quad G(u) \le 0$$

at the best available parameter estimate $\hat{p}$. Here, $G : \mathbb{R}^{n_u} \to \mathbb{R}^{n_G}$ is an inequality constraint function modeling the domain of realizable inputs.
(2) Implement the control u^* and collect measurements.
(3) Solve the parameter estimation problem (1) and store the new parameter estimate p^*.
(4) Stop if $\Phi(V(u^*, p^*)) < \text{TOL}$ for a desired accuracy tolerance TOL.
(5) Set $\hat{p} \leftarrow p^*$ and $\Sigma_0 \leftarrow V(u^*, p^*)$ and continue with Step 1.

Clearly, in the above outlined optimal experiment design procedure, the choice of the scalar design criterion Φ can have a large influence on how the above identification procedure performs. Examples for traditional designs are the A-criterion, E-criterion, and D-criterion, which aim at minimizing the trace, maximum eigenvalue, or determinant of the variance–covariance matrix, respectively. However, these choices are rather ambiguous and, in particular, in the literature on traditional optimal experiment design approaches there is often no advice on how to systematically refine the design criterion if the above identification loop is repeated more than once. This is in contrast to economic optimal experiment (Houska et al., 2015). Here, the underlying assumption is—in the easiest case—that our ultimate goal is to solve an optimization problem of the form:

$$u^*(p) \in \operatorname*{argmin}_u F(u,p) \quad \text{subject to} \quad G(u) \le 0, \tag{2}$$

whose objective function $F(\cdot, p) : \mathbb{R}^{n_u} \to \mathbb{R}$ depends on the unknown parameter p. The inequality constraint function $G : \mathbb{R}^{n_u} \to \mathbb{R}^{n_G}$ is assumed to be independent of p. Clearly, if we solve Problem (2) based on a parameter estimate instead of the exact but unknown value, we will in general obtain an optimality gap. Mathematically, this optimality gap can be defined as:

$$\Delta(p) := F(u^*(p), p_{\text{nature}}) - F(u^*(p_{\text{nature}}), p_{\text{nature}}),$$

where p_{nature} denotes the exact but unknown parameter. Now, the aim of the identification procedure is to determine the parameter