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Necessary condition for applying experimental design criteria to global sensitivity analysis results

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ABSTRACT

Conventional techniques for optimal experimental design are based on local sensitivity analysis to quantify parameter effects on the output. However, one of the key challenges for experimental design is that the local sensitivity is dependent on the unknown parameter values for a nonlinear model. This problem can be addressed if the sensitivity matrix, used in experimental design, could be computed by global sensitivity analysis techniques rather than local sensitivity analysis methods. However, not all existing global sensitivity analysis measures can compute such a sensitivity matrix. This paper presents a necessary condition for integrating global sensitivity analysis with experimental design criteria, i.e., the design criterion of the global sensitivity matrix reduces to the one applied to the local sensitivity matrix if the parameter uncertainty range tends to zero. Four different sensitivity measures are analyzed using this condition and the results are illustrated in a detailed case study where a comparison with local design and Bayesian design is made.

1. Introduction

Optimal experimental design has attracted a significant amount of attention due to the increasing use of model-based techniques in process systems engineering (Atkinson & Bogacka, 1997; Bandara, Schloder, Eils, Bock, & Meyer, 2009; Faller, Klingmuller, & Timmer, 2003; Gadkar, Gunawan, & Doyle, 2005; Galvanin, Macchietto, & Bezzo, 2007; Zhang & Edgar, 2008). Experimental design determines experimental conditions, e.g., input profiles and sampling times, such that the information content of the generated data is maximized for parameter estimation (Franceschini & Macchietto, 2008; Pronzato, 2008).

Optimal experimental design procedures generally involve two key components: (1) some form of information that determines how factors, that can be changed in an experiment, affect the outputs of a system and (2) an experimental design criterion which quantifies the information from (1) such that the quality of two designs can be directly compared.

For linear models, the parameter effect is usually characterized by the design matrix and a variety of experimental criteria on the design matrix have been developed. These criteria are named alphabetically (Kiefer, 1959, 1974) and called as the alphabetical experimental criteria. Every one of these criteria is a real function of the cross product of the design matrix for a linear system. The main advantage of using these experimental design criteria is that the criterion value is directly related to the quality of the parameter estimates.

The alphabetical experimental criteria are also locally applicable to nonlinear models via linearization. The local sensitivity matrix, i.e., the matrix containing the derivatives of how factors are affecting the outputs, is a substitute for the design matrix. Using such an approach, experiments can be designed by optimizing an alphabetical experimental criterion which is dependent upon the local sensitivity matrix. However, a main challenge of this approach is that the local sensitivity matrix is dependent on the unknown parameter values. A simple solution is the local design (Box & Lucas, 1959), which evaluates the local sensitivity matrix only at the nominal parameter values. Since the parameter uncertainty is neglected in the local design, the performance of the designed experiment is highly dependent on the parameter values used to evaluate the local sensitivity and the performance of the designed experiment cannot be guaranteed.

Bayesian design (Chaloner & Verdinelli, 1995) is one approach that addresses this challenge as the parameter uncertainty is directly taken into account. While Bayesian design involves application of an alphabetical criterion to a local sensitivity matrix, the design is performed for multiple values of the parameters and an expectation of the criterion over the parameter uncertainty is optimized instead of the criterion evaluated at only one specific set of parameter values.

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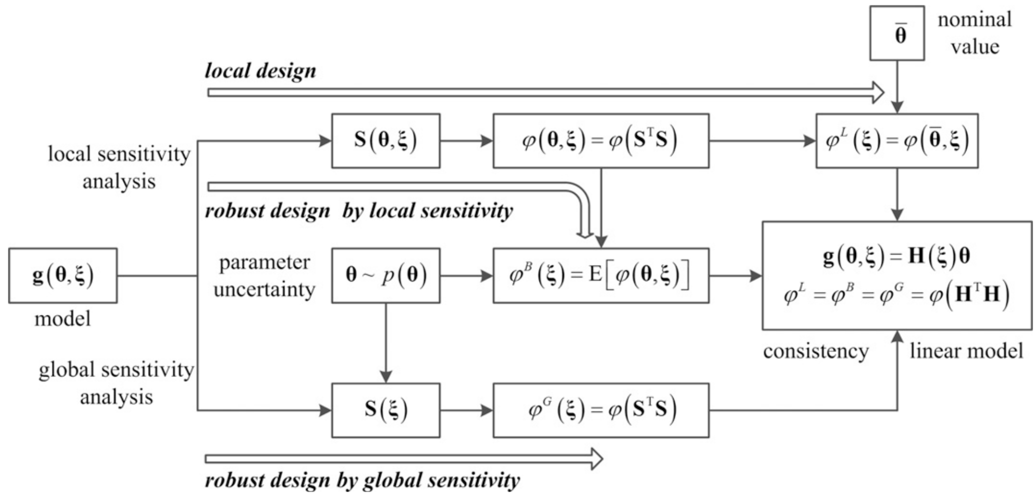

Fig. 1. Relationship of optimal experimental design via global sensitivity analysis with local design and conventional robust design via local sensitivity analysis. The notation of $\boldsymbol{\theta}$ is the parameter vector, $\boldsymbol{\xi}$ is the vector of design variables, $\mathbf{S}$ is the sensitivity matrix and φ is the alphabetical experimental criterion.

Another robust design approach developed recently is experimental design based on the global sensitivity matrix. Global sensitivity analysis (Saltelli, Ratto, Tarantola, & Campolongo, 2005; Saltelli, Tarantola, & Chan, 1999) takes the parameter uncertainty into account for calculation of the sensitivity value. This can address the main drawback of the local design, especially if it were possible to use the global sensitivity matrix to evaluate the design criterion instead of the local sensitivity matrix (Martinez, Cristaldi, & Grau, 2009; Rodriguez-Fernandez, Kucherenko, Pantelides, & Shah, 2007).

An overview of different experimental design strategies is provided in Fig. 1. Parameter uncertainty has no effect for linear experimental design, however, it is an essential component of experimental design involving a nonlinear model. Local design fails to take parameter uncertainty into account. While the conventional robust strategy of Bayesian design makes use of local sensitivities to quantify parameter effects on the outputs, parameter uncertainty is considered by repeatedly evaluating the sensitivity for nominal values that are sampled from a parameter uncertainty distribution. Bayesian design computes the mean value of the criterion function over the parameter uncertainty region. Contrary to this, global sensitivity analysis provides a different approach for robust design. Parameter uncertainty is taken into account while computing the parameter effects. The difference between the two robust design strategies results from the step at which parameter uncertainty is taken into account (see Fig. 1), i.e., Bayesian design computes a distribution of local sensitivities while the approach presented in this paper computes the sensitivities from a distribution of the parameter values.

While applying experimental design criteria to global sensitivity analysis results seems promising, it has to be carefully considered if and when such an approach can be used. The reason for this statement is that, unlike the local sensitivity, various global sensitivity measures exist and not all of them can be used for such a type of approach to experimental design. It is the goal of this work to propose a necessary condition which ensures that the existing alphabetical experimental design criteria can be applied to the results returned by global sensitivity analysis as is shown in Fig. 1. The necessary condition is called the consistency condition as it stipulates that the criterion function applied to the results returned by global sensitivity analysis should have the same value as the one applied to local sensitivity matrix when the parameter uncertainty range tends to zero. In this situation, the design by global sensitivity analysis is consistent with the one by local sensitivity analysis. The necessary condition also implies that the design involving global sensitivity analysis is consistent with the traditional linear design if the model is linear (see Fig. 1). The consistency condition is essential for extending the use of the common alphabetical criteria, which are derived for linear systems, to nonlinear models via sensitivity analysis. The condition is applied to four different global sensitivity measures in this work and a detailed comparison is made with the design based upon local sensitivity analysis, including both local design and Bayesian design. Significant advantages of the global approach are highlighted in a detailed case study.

The paper is organized as follows. A brief introduction to optimal experimental design and global sensitivity analysis is presented in Section 2. Application of global sensitivity analysis to optimal experimental design is presented in Section 3 and further demonstrated in an example in Section 4. Section 5 provides the conclusions.

2. Background

This section gives a brief review of optimal experimental design and global sensitivity analysis. This material serves as background information for the conditions presented in Section 3.

2.1. Optimal experimental design

Local sensitivity, which quantifies parameter effects on the outputs, plays a central role in conventional optimal experimental design procedures. An outline of the individual tasks involved in optimal experimental design via local sensitivity analysis is shown in Fig. 2.

Optimal experimental design involves a model of a dynamic system which is described by a set of ordinary differential equations including initial conditions. The data used for parameter estimation are generated by sampling the output vector $\mathbf{y}(t)$ at several time points $\{t_1, t_2, \ldots, t_l\}$. The output vector is assumed to have q entries, $\mathbf{y}(t) = [y_1(t), y_2(t), \ldots, y_q(t)]^{\mathrm{T}}$ resulting in a total of $m = q \cdot l$ data points. The outputs are dependent on the parameters, which are concatenated in the vector $\boldsymbol{\theta}$, and the experimental conditions, which are parameterized by a vector $\boldsymbol{\xi}$. Experimental conditions can include the input signals, the initial conditions, and the sampling time points. The function $\mathbf{g}(\boldsymbol{\theta}, \boldsymbol{\xi})$ in Fig. 2 is introduced to express the relationship between the model predictions and the