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Feasibility analysis of black-box processes using an adaptive sampling Kriging-based method

Fani Boukouvala, Marianthi G. Ierapetritou*

Department of Chemical and Biochemical Engineering, Rutgers University, Piscataway, NJ 08854, United States

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ABSTRACT

This paper presents a new approach for performing feasibility analysis over a multivariate factor space when the explicit form of a process model is lacking or when its evaluation is expensive. Specifically, two issues are addressed: feasibility evaluation of black-box processes using Kriging and development of an adaptive sampling strategy in order to minimize sampling cost, while maintaining feasibility space accuracy. Kriging is chosen as the interpolating technique for constructing a response surface of the feasibility function as a function of the uncertain parameters when a set of input–output data are available. The adaptive sampling strategy identifies critical regions and directs the search towards feasibility boundaries or where the Kriging prediction uncertainty is high. The average Kriging prediction error and cross-validation methods are used to validate the robustness of the produced model of the initial experimental design which is found to highly affect the final predicted feasible region.

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1. Introduction

Design and optimization under uncertainty is a key issue in process systems design, since often, decisions are made with limited knowledge about the process model and the variations in the environmental parameters (Swaney & Grossmann, 1985). In the last decades, several approaches have been proposed to systematically address uncertainty in process design based on different optimization formulations. The concept of process flexibility is one of the fundamental tools developed in order to express, quantify and evaluate the ability of a process to tolerate variations in its operating parameters or deviations of uncertain parameters from their nominal values. Using the concept of process flexibility one has the ability to calculate the maximum variations that a process can handle in order to remain in a feasible steady state. The problem of quantifying process flexibility has been well studied in the literature following the original formulation of Swaney and Grossmann (1985), where the effects of parameters that contain considerable uncertainty on the optimality and feasibility of a chemical process were studied. The objective of solving such problems was to ensure optimality and feasibility of operation for a given range of uncertain parameter values, by identifying the size of the feasible region of operation. Process flexibility is an important component of the operability characteristics of a process and it is formally defined as the capability of a design to operate feasibly under uncertain conditions. Mathematical formulations and indices have been developed to quantify flexibility. In order, however, to investigate how flexible a process is under variations during operation, the feasibility of a process must be verified within the space defined by the range of uncertain conditions.

Even though significant effort has been devoted in literature to develop or improve approaches and metrics for quantifying the feasibility of processes described by model equations (Floudas & Gumus, 2001; Ierapetritou, 2001; Pistikopoulos & Ierapetritou, 1995; Pistikopoulos, 1995; Straub & Grossmann, 1993; Vishal & Marianthi, 2003), fewer attempts have been made in the area of feasibility analysis of processes where closed form models are not available (black-box) (Banerjee & Ierapetritou, 2002). It is often the case that the explicit form of the model connecting the input parameters to the output is not available, while the only knowledge of the system consists of a set of noisy output values at different operating conditions. In Banerjee and Ierapetritou (2002, 2003) and Banerjee, Pal, and Maiti (2010), High Dimensional Model Representation methodology (HDMR) is used for input–output mapping of black-box processes, where the design under uncertainty problem is then solved. In Banerjee and Ierapetritou (2005), the feasible region is considered as an object and shape reconstruction techniques are used to approximate the feasible parameter space. The key to using black-box methods for performing feasibility analysis lies in balancing the need to minimize expensive and time consuming sampling with the necessity

* Corresponding author. Tel.: +1 732 445 2971; fax: +1 732 445 2581.
E-mail addresses: marianth@rutgers.edu, marianth@soemail.rutgers.edu (M.G. Ierapetritou).

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of accurately mapping the feasible region and strictly avoiding overprediction.

In this work, the performance of a different black-box interpolating technique – Kriging – is evaluated for performing feasibility analysis. Kriging is a data-driven methodology that has a long history in many fields such as geology (Cressie, 1993a), statistics and optimization – where it is referred to as the Design and Analysis of Computer Experiments (DACE) stochastic process model (Jones, Schonlau, & Welch, 1998). In Kriging, the prediction at a test point is expressed as a weighted sum of observed function values at sampling points that fall within a set interval around it. From a statistical viewpoint, Kriging is a stochastic approach that provides – for each test point – a mean value (predictor) as well as a measure of possible error in the prediction (variance). This approach is chosen for two reasons, first because it has been shown that it requires fewer function evaluations than other competing methods (Jones et al., 1998) and second because the calculated variance for each test point can identify regions where subsequent sampling is required (Davis & Ierapetritou, 2007).

One of the main limitations of sampling based approaches is that there is no a priori knowledge of the number of sampling points that are needed or the location of those points in order to provide maximum information for the accurate prediction of the output surface (Davis & Ierapetritou, 2010). The literature of sampling based techniques for optimization focuses on optimizing both the number and the spatial arrangement of sampling points for the identification of a global optimum (Simpson, Lin, & Chen, 2001). Random sampling is an easily implementable approach but it may lead to an inaccurate representation of the feasible region as well as a poor model development. Stratified sampling refers to the implementation of any algorithm that samples subsets of the test points based on a stratification rule. This type of sampling guarantees more uniform sampling compared to random sampling. A different strategy known as systematic sampling refers to methodologies that incorporate a simple heuristic rule for the identification of the number of samples chosen for each sampling vector. A characteristic example is centroid based sampling which is based on the geometry of Delaunay triangles (Davis & Ierapetritou, 2010). Finally, cluster sampling leads to a non-uniform sampling set by identifying regions of high interest and excluding regions that do not provide useful information about the system performance. A more extensive literature review of different types of sampling techniques for optimization can be found in (Davis & Ierapetritou, 2010; Simpson et al., 2001).

The efficiency of sampling based techniques for performing black-box feasibility analysis has not been addressed so far in the literature. The designation of "black-box feasibility analysis" will be referred in this paper to describe the procedure of solving the flexibility test problem and the mapping of the feasible region of a process for which the closed form expression of the model and constraints are not available. In this work, an adaptive sampling technique which makes use of ideas from existing sampling techniques for optimization is tailored to the nature of the described problem and is developed for the accurate feasibility space mapping reducing the required number of samples.

The remaining of the paper is organized as follows. The mathematical formulation of process flexibility is described in Section 2. Section 3 describes the methodology used in this work to perform feasibility analysis consisting of Kriging interpolation and adaptive sampling, while Section 4 presents the Model Validation. Following, Section 5 is comprised of a number of examples through which the performance of the proposed methodology is demonstrated. An application of the proposed methodology is described in Section 6 through the feasibility analysis of a roller compaction process for pharmaceutical powders. Finally the paper concludes with a discussion of the results as well as future directions of the presented work.

2. Process feasibility problem

In the literature flexibility is defined as the ability of a design to maintain feasible steady state operation for a range of uncertain conditions that may be encountered during operation. The quantification of process flexibility is achieved through the formulation of the flexibility test problem, introduced by Swaney and Grossmann (1985). According to the methodology introduced in this work, the problem is represented as a max–min–max formulation, where, for a specific design and given ranges of the uncertain parameters, the feasible region is defined. The flexibility was then quantified by the flexibility index (FI), which represented the maximum allowed deviation of uncertain parameters from their nominal values, such that feasible operation could be guaranteed by changing the control variables. A series of papers dealing with flexibility analysis and the formulation and optimization of processes under uncertainty were published in the following years, most of them, however, required known process models and relied on particular convexity assumptions (Floudas & Gumus, 2001; Grossman & Floudas, 1987; Vishal & Marianthi, 2002, 2003).

The general problem that is considered for flexibility analysis has the following form:

$$\begin{aligned}&\min_{d,z,x} f(d, z, x, \theta)\\&\text{s.t.}\\&h(d, z, x, \theta) = 0\\&g(d, z, x, \theta) \leq 0\\&d \in R^n, \quad z \in R^q, \quad x \in R^q, \quad \theta \in T\end{aligned} \tag{1}$$

where d corresponds to the design variables, z and x represent the control and state variables, respectively, θ corresponds to the uncertain parameters of the process, h is process equations describing the system, g corresponds to bounds on variables, design specifications or logical constraints, f is the objective function to be minimized, and $T = \{\theta | \theta^L \leq \theta \leq \theta^U\}$. Eliminating the equality constraints h by expressing all state variables in terms of d, z and θ, the objective function of the feasibility problem (1) becomes:

$$\begin{aligned}&\min_{d,z} f(d, z, \theta)\\&\text{s.t.}\\&y(d, z, \theta) \leq 0\\&d \in R^n, \quad z \in R^q, \quad \theta \in T\end{aligned} \tag{2}$$

Solving (2) determines whether for a given design d and values of uncertain parameters θ the control variables z can be adjusted to satisfy all the necessary constraints and attain feasibility. This can be accomplished if for a given value of θ, all constraints $y_j \leq 0$ are satisfied. By defining the feasibility function $\psi(d, \theta) = \min_z \max_{j \in J} \{y_j(d, z, \theta)\}$, where J is the set of inequality constraints, the controls are selected such that the maximum y_j is minimized. This optimization problem can be further transformed into the following form by introducing the scalar parameter u such that:

$$\begin{aligned}&\psi(d, \theta) = \min_{u,z} u\\&\text{s.t.} \quad y_j(d, z, \theta) \leq u, \quad j \in J\end{aligned} \tag{3}$$

In order to determine whether feasible operation can be attained in the parameter uncertainty range T, it is clear that $\psi(d, \theta) \leq 0$ for all $\theta \in T$. In its most compact form, the flexibility test problem can be represented as a max–min–max formulation, since it is sufficient to ensure whether the maximum value of the feasibility function is less or equal to zero in order to maintain feasible operation.

$$\chi(d) = \max_{\theta \in T} \min_{z} \max_{j \in J} g_j(d, z, \theta) \tag{4}$$