Contents lists available at SciVerse ScienceDirect

Chemical Engineering Research and Design

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Response surface methodology with prediction uncertainty: A multi-objective optimisation approach

Guoyi Chi[a], Shuangquan Hu[a], Yanhui Yang[a], Tao Chen[a,b,*]

[a] School of Chemical and Biomedical Engineering, Nanyang Technological University, 62 Nanyang Drive, Singapore 637459, Singapore
[b] Division of Civil, Chemical and Environmental Engineering, University of Surrey, Guildford GU2 7XH, UK

ABSTRACT

In the field of response surface methodology (RSM), the prediction uncertainty of the empirical model needs to be considered for effective process optimisation. Current methods combine the prediction mean and uncertainty through certain weighting strategies, either explicitly or implicitly, to form a single objective function for optimisation. This paper proposes to address this problem under the multi-objective optimisation framework. Overall, the method iterates through initial experimental design, empirical modelling and model-based optimisation to allocate promising experiments for the next iteration. Specifically, the Gaussian process regression is adopted as the empirical model due to its demonstrated prediction accuracy and reliable quantification of prediction uncertainty in the literature. The non-dominated sorting genetic algorithm II (NSGA-II) is used to search for Pareto points that are further clustered to give experimental points to be conducted in the next iteration. The application study, on the optimisation of a catalytic epoxidation process, demonstrates that the proposed method is a powerful tool to aid the development of chemical and potentially other processes.

Keywords: Design of experiments; Gaussian process regression; Heterogeneous catalysis; Kriging; Model uncertainty; Response surface methodology

1. Introduction

Response surface methodology (RSM) is a widely used technology for rational experimental design and process optimisation in the absence of mechanistic information (Box and Draper, 1987; Myers and Montgomery, 1995). RSM initiates from design of experiments (DoE) to determine the factors' values for conducting experiments and collecting data. The data are then used to develop an empirical model that relates the process response to the factors. Subsequently, the model facilitates to search for better process response, which is validated through experiment(s). The above procedure iterates until an optimal process is identified or the limit on experimental resources is reached. RSM has seen diverse applications in almost every area of scientific research and engineering practice, including the development of chemical and biochemical processes (Agatonovic-Kustrin et al., 1998; Baumes et al., 2004; Dutta et al., 2004; Hadjmohammadi and Kamel, 2008; Shao et al., 2007; Tang et al., 2010; Yan et al., 2011a,b).

In traditional RSM, the first- or second-order polynomial function is adopted for empirical modelling. However, the restrictive functional form of polynomials has long been recognised as ineffective in modelling complex processes. Progress in adopting more flexible models in RSM includes artificial neural networks (ANN) (Agatonovic-Kustrin et al., 1998; Baumes et al., 2004; Dutta et al., 2004; Shao et al., 2007), support vector regression (SVR) (Hadjmohammadi and Kamel, 2008; Serna et al., 2008), and more recently Gaussian process regression (GPR) (Tang et al., 2010; Yan et al., 2011a,b; Yuan et al., 2008). GPR, also known as kriging model with slightly different formulation, has been accepted as a powerful modelling tool in various fields, in particular in process systems engineering (Ge and Song, 2010; Grancharova et al., 2008; Likar and Kocijan, 2007). GPR is attractive partly because of the sound

* *Corresponding author at*: Division of Civil, Chemical and Environmental Engineering, University of Surrey, Guildford GU2 7XH, UK. Tel.: +44 1483 686593; fax: +44 1483 686581.
E-mail address: t.chen@surrey.ac.uk (T. Chen).
Received 25 February 2011; Received in revised form 23 September 2011; Accepted 12 December 2011
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doi:10.1016/j.cherd.2011.12.012