Computers and Chemical Engineering 108 (2018) 250–267

Contents lists available at ScienceDirect

Computers and Chemical Engineering

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

Review

Advances in surrogate based modeling, feasibility analysis, and optimization: A review

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ARTICLE INFO

Article history:
Received 5 June 2017
Received in revised form 5 September 2017
Accepted 19 September 2017
Available online 21 September 2017

Keywords:
Surrogate models
Derivative-free optimization
Feasibility analysis
Sampling
Model selection

ABSTRACT

The idea of using a simpler surrogate to represent a complex phenomenon has gained increasing popularity over past three decades. Due to their ability to exploit the black-box nature of the problem and the attractive computational simplicity, surrogates have been studied by researchers in multiple scientific and engineering disciplines. Successful use of surrogates shall result in significant savings in terms of computational time and resources. However, with a wide variety of approaches available in the literature, the correct choice of surrogate is a difficult task. An important aspect of this choice is based on the type of problem at hand. This paper reviews recent advances in the area of surrogate models for problems in modeling, feasibility analysis, and optimization. Two of the frequently used surrogates, radial basis functions, and Kriging are tested on a variety of test problems. Finally, guidelines for the choice of appropriate surrogate model are discussed.

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http://dx.doi.org/10.1016/j.compchemeng.2017.09.017
0098-1354/

1. Introduction

The problem discussed in the paper is assessing the performance of surrogates on the deterministic function $f: R^d \to R$; where the input vector is $X = (x_1, x_2, \ldots, x_d)$, d is the number of dimensions of $X^L \leq X \leq X^U$ the problem, and there is a single output y. The input vector X has known lower and upper bounds

Additionally, some constraints $f_j \leq 0$, $j \in J$ where J is the set of all constraints, may be present. It is assumed that evaluation of the function as well as constraints is computationally expensive and the symbolic form of the function and that of one or more constraints is unknown. From this assumption, it follows that the analytical form of the derivatives is also unavailable. Surrogate modeling addresses this problem by obtaining a function $\hat{f}(X)$ that approximates the function f.

This problem occurs frequently in multiple engineering and scientific disciplines where complex computer simulations or physical experiments are used. In these cases, obtaining more data means additional experiments and thus it results in significant material or economic cost as well as highly non-trivial computational expense. As a result, it is difficult to obtain an analytical form of the objective function or that of the derivatives. Deriving this information from surrogate $\hat{f}(x)$ is relatively easier because its analytical form is known and it is cheaper to evaluate. Several applications of surrogates to address this type of problems can be found in the literature. For example, (Anthony et al., 1997), (Balabanov and Haftka, 1998), use polynomial, linear response surfaces in aircraft design. Artificial neural networks (ANN) is used for process modeling (Meert and Rijckaert, 1998), process control (Bloch and Denoeux, 2003), (Mujtaba et al., 2006), and for optimization (Fernandes, 2006), (Henao and Maravelias, 2011). Kriging is used for process flowsheet simulations (Palmer and Realff, 2002), design simulations (Yang et al., 2005), (Prebeg et al., 2014), pharmaceutical process simulations (Jia et al., 2009), and feasibility analysis (Rogers and Ierapetritou, 2015). Radial basis functions (RBF) is used for feasibility analysis (Wang and Ierapetritou, 2016) and parameter estimation (Müller et al., 2015). It can be observed from the $\hat{f}(x)$ applications listed above that there are multiple approaches proposed in literature to obtain a surrogate.

Several prior reviews discuss these approaches and related developments in the field of surrogate models. Surrogate models and their potential use in simulations is discussed by (Barton, 1992). They discuss polynomial response surface, spline interpolation, radial basis functions, regression models, and Kriging surrogates. With the focus on modeling and prediction for engineering design, (Simpson et al., 1997) review stationary sampling designs, polynomial response surface methods, Kriging and robust methods. (Jin et al., 2001) studied performance of polynomial regression, multivariate adaptive regression splines, radial basis functions, and Kriging surrogates under multiple criteria such as efficiency, robustness and model simplicity. Motivated from applications in aerospace systems, (Queipo et al., 2005) discuss surrogate based optimization and sensitivity analysis, sampling strategies and surrogate model validation. (Barton and Meckesheimer, 2006) discuss surrogates for guiding optimization of simulations. In this context of guiding search towards optimum, they classify surrogates as local surrogates that are updated within an iterative framework and global surrogates that are fitted only once and the search proceeds using the same surrogate thereafter. For the purposes of design optimization, (Wang and Shan, 2007) provide an overview of surrogate models. Their focus is mainly on solving optimization problems such as global optimization, multi-objective optimization, and probabilistic design optimization. Motivated from computationally intensive aerospace designs, (Forrester and Keane, 2009) discuss details of surrogate modeling methodology focusing on sampling, surrogate model building, and validation. They discuss surrogates such as polynomial interpolation, RBF, Kriging and support vector regression and their advantages and disadvantages for achieving better prediction accuracy. (Razavi et al., 2012) investigate the potential of surrogate modeling techniques with a focus on the use of surrogates in water resources applications. They provide an excellent review on use of surrogates in water resources. (Nippgen et al., 2016) review surrogate modeling strategies from a broader point of view by classifying those as data-driven, projection-based and multi-fidelity surrogate modeling strategies. They focus on potential of using surrogates for applications in groundwater modeling. (Haftka et al., 2016) discuss in detail, several strategies for global optimization using surrogates, criteria for local and global searches from the point of view of parallelization. It is important to note that with respect to applications, the problems requiring surrogates can be classified in to three classes. The first class of problems is the most fundamental use of surrogates i.e. prediction and modeling. The second class of problems is commonly known as derivative-free optimization (DFO) where the objective function to be optimized is expensive and thus derivative information is unavailable. The third class of problems is feasibility analysis where the objective is also to satisfy design constraints. Prior reviews discuss applications of surrogate models for only one or two of these three classes. This review emphasizes that there is a significant difference between using surrogates for each of these three classes of problems and provides a comprehensive understanding of surrogate models for all three classes of problems mentioned. There has been a growing interest in model selection methodologies for regression models where the aim is to choose the best model from a given set of models. This problem has many practical uses in cases where the surrogate model does not generalize well on the test set, a phenomenon commonly known as overfitting or when there are too many input variables that might contain redundant information. In such cases, it is important to select most relevant variables in order to build simple yet effective surrogate models. Even though model selection is popular in the field of statistics for over 50 years, prior reviews in the con-