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Value of information method for optimization and experimental design using surrogate models

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Abstract

Experimentation is required for modeling empirical functions and optimization. In manufacturing, experiments are costly and time-consuming, thereby limiting the number of function evaluations. This paper describes a value of information method for experimental design and optimization using surrogate modeling. Value of information is defined as the absolute difference between optimal value before experiment and the expected optimal value after experiment, or, the expected improvement in the optimum after experiment. The value of information based experimental design performs better than the traditional statistical design of experiments such as Taguchi orthogonal arrays, and central composite design, especially in three or more dimensions.

Keywords: Value of information; Design of experiments; Surrogate models; Optimization; Uncertainty

Empirical functions are typically evaluated using experimentation over the range of process parameters. Examples in the manufacturing literature are surface roughness modeling in milling [1–3], turning [4–5], and laser assisted machining [6], tool life modeling [7–9], geometric error in grinding [10–11], material removal rates in electric discharge machining (EDM), and polishing [12–14]. The goal of experimentation is to find the process parameters for optimizing the objective function, such as material removal rate or surface roughness. The experimental design is typically carried out using design of experiment (DOE) methods for optimizing the number of experiments required to achieve a desired output [15,16]. However, traditional DOE methods such as Taguchi orthogonal arrays, central composite design, or factorial design are sub-optimal for two reasons. First, DOE typically requires a fixed number of experiments which are decided prior to any testing and do not take into account the cost of performing the experiments. For example, for three or more process variables, the experimental cost for tool life modeling may be large. Second, DOE does not consider the economic impact of uncertainty reduction to the decision maker and the uncertainty in the experimental outcomes.

To address these limitations, this paper describes a value of information method for experimental design and optimization of empirical functions using surrogate models. Value of information (*VOI*) is defined as the absolute difference between optimal value before experiment and the expected optimal value after experiment, or, the expected improvement in the optimum after experiment [17,18]. The fundamental principle governing the value of information method is that an experiment is only worthwhile if the value gained from the experiment is more than the cost of performing the experiment [17]. An experiment should be performed at the process variables which add the most (expected) value. The approach is advantageous over traditional DOE as it considers the importance of uncertainty reduction to the decision maker by assigning a value to the information gained from an experiment, takes into

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account the underlying objective of experimentation, and the probabilistic nature of the experimental results and its impact on the objective function [17]. The value of information is a normative and robust figure of merit as it balances local and global search by exploiting regions where the cost function is minimized (local) and by exploring regions where the prediction uncertainty is high (global) [19,20]. The value of information method has not yet been applied for experimental design in manufacturing; the main contribution of this paper is to demonstrate the method for experimental design and optimization using surrogate models. A generalized framework is presented and potential applications in the manufacturing domain are listed.

1. Surrogate modeling

Surrogate models offer an attractive solution for modeling empirical functions in the absence of any physics based models. Examples of surrogate models are kriging, Gaussian process regressions, support vector machines, radial basis functions, and polynomial response surface [21,22]. For brevity, the reader is referred to [21,22] for mathematical modeling and the theory behind developing the surrogates. The choice of the surrogate model depends on the application and the experimental uncertainty. To illustrate, kriging is an exact interpolator for predicting the distribution of a random field at unobserved locations and is applicable in situations where the experimental outcomes are deterministic or the uncertainty is negligible. In applications such as surface roughness modeling in machining, multiple measurements can be made along the machined surface and the experimental outcome taken as the average value of the measurements. In this case, kriging models the expected value of the optimization variable of interest. An alternative approach is modeling using Gaussian process regression which takes into account the experimental uncertainty in the variable of interest.

Let y be a one dimensional objective function of interest, dependent on variable x. For example, the function y can be tool wear, machining cost, or surface roughness in milling and x can be the process parameters such as cutting speed, or feed rate. The objective is to optimize the number of experiments required to find the minimum value of y and the corresponding value of x. Note that the true location of the optimum is not known, and therefore, uncertain. Figure 1 shows the kriging (left) and Gaussian process (right) prediction after four experiments. The solid line represents the prediction mean and the dotted line shows the $\pm 3\sigma$ bounds, where σ is the standard deviation. The surrogate model parameters can be tuned to maximize the likelihood of experimental results. Based on the four experimental results, the current optimum value, $y_{\min}$, is 7.2 at $x = 1.8$; the optimum is taken as the minimum from the experimental results. Note that although the paper uses kriging predictions, shown in Figure 1 (left), to calculate value of information, the procedure is applicable to alternative models such as Gaussian process regression.

2. Experimentation

This section describes the steps to calculate the value of information for experimental design. The first step is to investigate if any additional experimentation is necessary. The value of perfect information ($VOPI$), also called as the value of clairvoyance, gives the value of eliminating uncertainty through experimentation [17,23]. $VOPI$ is the expected improvement from the current optimum ($y_{\min} = 7.2$) if the true function was known with certainty. In simple words, $VOPI$ gives the maximum value the user would be willing to pay a clairvoyant to know the true optimum. $VOPI$ places an upper bound on the costs of experimentation; experimentation is not necessary if the costs of the experiments exceed the $VOPI$. For a minimizing function, $VOPI$ is given by Eq. (1).

$$VOPI = \text{optimal value before experiment} - E(\text{optimal value after perfect information}) \quad (1)$$

For the function under consideration, $VOPI$ was calculated as follows. Random samples were drawn from the kriging predictions shown in Figure 1 (left) using the mean,

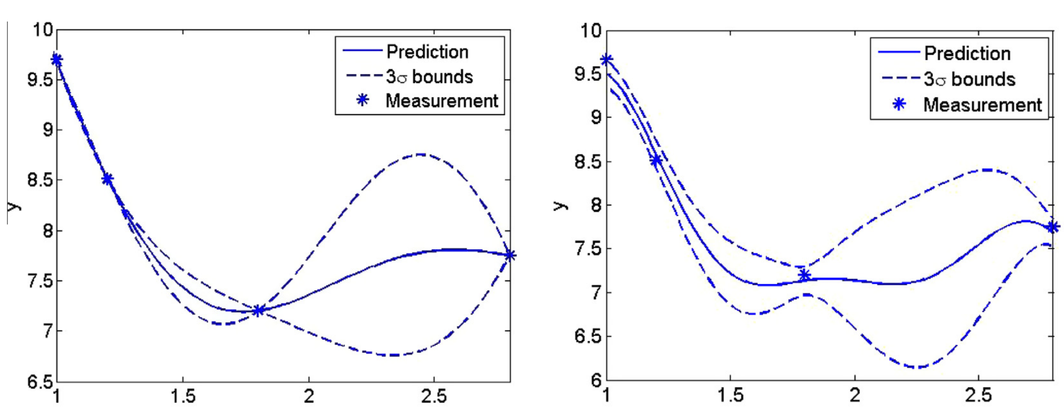

Figure 1. Surrogate model predictions after four experiments using kriging (left) and Gaussian process regression (right). The experimental results are denoted by '*'.