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USING RADIAL BASIS FUNCTIONS TO OPTIMIZE BLACK-BOX FUNCTIONS WITH NOISY OBSERVATIONS

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ABSTRACT

This study proposes a new global optimization algorithm (TRIM) for expensive black-box functions subject to evaluation noise. We use radial basis functions (RBFs) as surrogate and extend the Stochastic Response Surface (SRS) method to functions with noisy evaluations. To balance the trade-off between exploration, exploitation and accuracy of evaluated points, we sequentially select the evaluation points based on three specific metric functions. Case studies show that the proposed algorithm is more effective in finding the optimal solution than other alternative methods.

1 INTRODUCTION

Global optimization for stochastic black-box expensive functions has received much of attention because of its wide applications in different areas including simulation optimization and manufacturing optimization (e.g., Huang et al. 2006). A big challenge for this type of problem is that an algorithm needs to produce a satisfying solution in a very limited budget since the function evaluation is expensive.

Metamodeling is a common technique that can be employed to optimize expensive functions, where a response surface (i.e., surrogate) model is constructed to support the search for the global minimum(Jones et al. 1998; Huang et al. 2006; Regis and Shoemaker 2007; Frazier et al. 2009; Quan et al. 2013). The purpose of using a surrogate is to reduce the number of function evaluations and one key step is to achieve the balance between exploration and exploitation (e.g., expected improvement (EI) in a kriging surrogate and weighted score in an RBF surrogate).

When the evaluation is noisy, besides exploration and exploitation, the accuracy at each evaluated point should also be considered in the sampling strategies. Algorithms need to decide when to perform replications at some points to alleviate the evaluation noise. In a stochastic kriging model, the co-variance matrix is the summation of two parts: the *extrinsic* uncertainty term as in a deterministic kriging model and the *intrinsic* uncertainty due to the evaluation noise (Ankenman et al. 2010) and acquisition functions (e.g., modified expected improvement (MEI)) can be defined accordingly to indicate when to perform replications. In the research, we try to generalize the general SRS framework to optimize noisy functions using RBFs as surrogate.

2 THE PROPOSED ALGORITHM

We consider the optimization problem, $x^* = \arg\min_{x \in X} f(x)$, where $X = [a, b]^d$ and $f(x)$ is a black-box function. The evaluation noise at x is normally distributed with mean 0 and (unknown) standard deviation. As with other surrogate algorithms, we sequentially select the next evaluation point and update the surrogate information after each iteration. In this algorithm, the scheme for selecting the next evaluation point is as follows: (a) select a point A from randomly generated points based on the first stage metric $\Psi_1(x)$; (b) select a point B from the evaluated points set based on the second stage metric $\Psi_2(x)$; (3) compare points A and B based on the third stage $\Psi_3(x)$ and finally make a decision on whether to evaluate the new point A or perform a replication at point B. The overall framework of our algorithm is given in Figure 1.

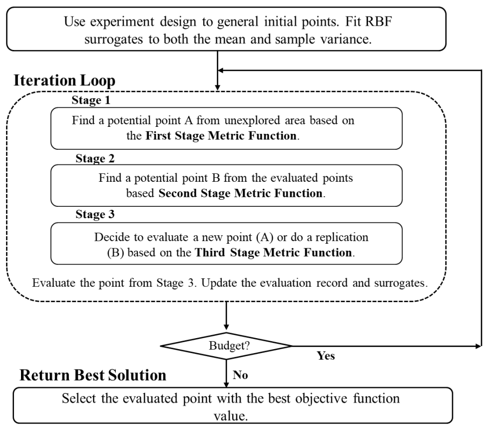

Figure 1. Diagram of the algorithm.

Table 1. Performance of the Algorithm.

	EQI		TSSO		TRIM	
	MEAN	STD	MEAN	STD	MEAN	STD
|x-x*|	0.318	0.253	0.312	0.252	0.053	0.120
|f(x)-f(x*)|	1.669	0.998	1.669	0.991	0.416	0.435

3 NUMERICAL RESULTS

We verify the performance of the RBF based algorithms with two kriging based algorithms TSSO and EQI (Quan et al. 2013, Picheny et al. 2013). We consider the following 2-d function,

$$f(x_1,x_2) = -5(1-(2x_1-1)^2)(1-(2x_2-1)^2)(3+2x_1)\left(0.05^{(2x_1-1)^2} - 0.05^{(2x_2-1)^2}\right).$$

The feasible domain is $[0,1]^2$ and the standard deviation of observation noise at (x_1,x_2) is $1.2x_1$. Table 1 presents the performance of TSSO, EQI, and the proposed TRIM algorithm with 1000 function evaluations and 100 trials. The initial settings and numerical results of TSSO and EQI are taken from literature. The initial settings of our algorithm follow the suggestions given in Regis and Shoemaker (2007). “MEAN” and “STD” in the table represent the mean and standard deviation of the distance from the returned solution to the true optimum of 100 trials. The results in Table 1 show that the proposed algorithm is more effective and return a solution closer to the true optimum.

Besides the above 2-d example, we will also compare the proposed algorithm with TSSO, EQI and CKG (Frazier et al. 2009) on four high dimensional functions: 3-d Hartman, 6-d Hartman, 10-d Michalewicz, and 20-d Ackley at three noise levels (Low, Medium, High).

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