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Using adaptive multi-accurate function evaluations in a surrogate-assisted method for computer experiments

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ABSTRACT

In many computer experiments, surrogates are used to assist in searching for certain target points. If the surrogates are defined by response function values evaluated by costly iterative processes, the computational burdens may impede the efficiency of regular surrogate-assisted methods. Instead of computing the fully convergent response function values, we propose to control the function evaluation iterations dynamically to save time on function evaluations without degrading the overall performance. Our new algorithms adaptively determine whether each of the function evaluation iterations should be paused, kept running, or restarted; we then use the approximate function values with various levels of accuracy to construct the surrogates. The numerical results show that the proposed algorithms achieve significant savings when solving super-level set searching problems that involve identifying positive Lyapunov exponents of a dynamical system.

1. Introduction

The rapid growth of computer capability has stimulated researchers to use mathematical models to simulate complex experiments on their computers. However, some computer experiments may require huge computational costs, consequently limiting their use. It is thus important to design computer experiments carefully to explore an experimental region efficiently.

This article focuses on finding a super-level set in computer experiments. A super-level set is defined as

$$\{\mathbf{x} | \mathbf{x} \in \mathcal{S} \subseteq \mathbb{R}^n \text{ and } f(\mathbf{x}) \in \mathbb{R} > a\}, \tag{1}$$

where $\mathcal{S}$ is a given experimental region, $f(\mathbf{x})$ is the response function of the computer experiments, and a is a given constant. A point $\mathbf{x}$ that belongs to the super-level set is called an *effective point*. Furthermore, we assume that the response function values are computed by iterative processes in terms of the (virtual) time step t:

$$f(\mathbf{x}) = \lim_{t \to \infty} f(\mathbf{x}, t). \tag{2}$$

Approaches used to solve such super-level finding problems can be affected by the properties of the response functions. In this article, we consider the following problems: (i) the function $f(\mathbf{x})$ is expensive to be evaluated, and (ii) the derivative of $f(\mathbf{x})$ is unknown. Consequently, the main goal of this article is to develop algorithms equipped with the following features:

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(i) we use a surrogate-assisted method that requires only the function values, rather than the derivative of $f(\mathbf{x})$, to guide the search for the effective points, and (ii) to construct the surrogates, we need to evaluate function values on certain experimental points. We use approximate response function values at different levels of accuracy adaptively to reduce the cost of function evaluations without degrading the overall performance.

Computer experiments with these types of response functions have been studied in several optimization contexts by using a couple of two different levels of accuracy (but without using multiple accuracy levels adaptively). For example, [1–3] consider surrogate construction problems where two solvers are used. One of the solvers is generally more accurate than the other one, but also more expensive to run. The authors of [1–3] study how to design cheaper computer experiments by using the two solvers, such that the resulting surrogate is similar to the one built using only the more accurate solver. In some circumstances, the solver itself may control the accuracy of the function values. In [4], a solver capable of very high accuracy is used for aerodynamic optimization computer experiments. Instead of using fully converged results all the time, partially converged data at a lower level of accuracy are used for surrogate constructions. Forrester et al. [5] modified the previous algorithm by combining it with the surrogate construction method proposed in [1]. These works demonstrate that we can achieve a higher level of efficiency for the overall algorithm by controlling the accuracy of the simulation in terms of the number of iterations in the evaluation processes. Note that the so-called "one-shot method" proposed in [6] also uses the idea of partial convergence. However, no surrogate is used in the one-shot method. Polak and Wetter [7] have extended the generalized pattern search algorithms to include a procedure that adaptively controls the accuracy of the response evaluation. From their numerical experiments, the efficiency of this control procedure is justified by significant reductions in the overall computation times.

Various surrogate-assisted methods have been proposed for various applications. In each iteration of such methods, surrogates that approximate the true yet unknown response surfaces are updated in each trial, and new experimental points are selected accordingly. The methods are continually iterated until all of the available computational resources have been consumed or until all the points satisfying certain criteria (e.g., optimal) have been found. For example in optimization problems, kriging [8], radial basis function [9], and surrogate management frameworks [10] have all been considered. In [11,12], the authors use surrogates that are based on an over-complete basis set in the search for parameter combinations for secure communication.

In this article, we consider the parameter combination problem described in [11] and [12], which can be formulated as the super-level search problems. Unlike the approach used in these two papers, which do not take into account the function evaluation iterations defined in Eq. (2), we study how approximate function values at multiple levels of accuracy can be used to improve the performance of the surrogate based algorithms. In particular, we consider the case where the super-level set is

$$\{\mathbf{x}|\mathbf{x} \in \mathcal{P} \subseteq \mathcal{S} \subseteq \mathbb{R}^n \text{ and } f(\mathbf{x}) \in \mathbb{R} > a\}. \tag{3}$$

Here, $\mathcal{P}$ stands for a grid domain that is feasible according to some physical constraints.

To solve the super-level problem defined by (2) and (3), we use the framework of surrogate-assisted methods. One key point for achieving efficiency is to construct the surrogates without running function evaluation processes to the limit. Therefore, we propose monitoring the function evaluation processes and using the approximate of function values dynamically at various levels of accuracy to construct the surrogates. An adaptive mechanism is proposed to control the function evaluation processes, determine the accuracy of function values, update surrogates, and select new experimental points. More specifically, we control the function evaluation iterations dynamically by combinations of pausing, keeping running, and restarting the process. We simultaneously monitor the function evaluation processes to see whether a so-called "metastable" criterion is satisfied before convergence. Once the metastable criterion is satisfied, the approximate function value at the corresponding level of accuracy will be used to update the surrogate. We compare the methods proposed here with the one proposed in [11], as they share the same surrogate framework but use distinct iterative control mechanisms. The numerical experiments show promise, with a 50%–70% computational cost savings.

The rest of this paper is organized as follows. In Section 2, we present the general framework of our algorithm. We discuss how to control the iterative function evaluation processes and how to integrate the intermediate results with the surrogate constructions. We also conduct convergence and complexity analysis of the algorithms. In Section 3, test problems are introduced and numerical results are presented. We conclude this paper in Section 4.

2. The proposed algorithms

We propose to solve the super-level set problem described in (2) and (3) by modifying the usual framework of surrogate-assisted search methods. One of the key points in such modifications is to understand the interplay between iterative processes of function evaluations, surrogate constructions, and target object functions. In this section, we will discuss how we can dynamically use the evaluated function values at different levels of accuracy to reduce the cost of constructing effective surrogates, thereby justifying the use of partially convergent function evaluations in the super-level set problem.

We begin our discussion by illustrating a general surrogate-assisted search algorithm in Algorithm 1.