Proceedings of the 2013 Winter Simulation Conference
R. Pasupathy, S.-H. Kim, A. Tolk, R. Hill, and M. E. Kuhl, eds.

AN ADAPTIVE RADIAL BASIS FUNCTION METHOD USING WEIGHTED IMPROVEMENT

Yibo Ji
Sujin Kim

Department of Industrial and Systems Engineering
National University of Singapore
119260, SINGAPORE

ABSTRACT

This paper introduces an adaptive Radial Basis Function (RBF) method using weighted improvement for the global optimization of black-box problems subject to box constraints. The proposed method applies rank-one update to efficiently build RBF models and derives a closed form for the leave-one-out cross validation (LOOCV) error of RBF models, allowing an adaptive choice of radial basis functions. In addition, we develop an estimated error bound, which share several desired properties with the kriging variance. This error estimate motivates us to design a novel sampling criterion called weighted improvement, capable of balancing between global search and local search with a tunable parameter. Computational results on 45 popular test problems indicate that the proposed algorithm outperforms several benchmark algorithms. Results also suggest that multiquadrics introduces lowest LOOCV error for small sample size while thin plate splines and inverse multiquadrics shows lower LOOCV error for large sample size.

1 INTRODUCTION

One common practice to optimize expensive functions is to build a metamodel and generate promising candidate points based on it. RBF models are widely used in metamodel-based global optimization because of their robustness and efficient construction achieved by simply solving a system of linear equations.

The literature on RBF model-based optimization has two main branches. Gutmann (2001) defined a bumpiness measure for an RBF model based on its seminorm. The other branch of the literature focuses on the better utilization of RBF model predictions and prediction uncertainties represented by the distance to the nearest evaluated point, see Regis and Shoemaker (2007), Regis (2011), and Jakobsson et al. (2010). Although Wendland (2005) reviewed a pointwise error bound for the RBF model predictions, but its dependence on a parameter related to the unknown true function restricts its applications in metamodel-based optimization. We believe that a better error estimate may guide the algorithm to conduct searches more wisely.

2 DESCRIPTION Of ALGORITHM

Figure 1 depicts the general structure of the proposed algorithm, WIRBF. This paper considers augmented RBF models, which are linear combinations of both radial basis functions and polynomials with certain degree. Such RBF models accommodate a wide range of basis functions, such as cubic and thin plate splines. We update RBF models using the matrix inverse lemma (Golub and Van Loan 1996), which avoids inverts the interpolation matrix of RBF models whenever additional points are available. The same lemma helps us obtain a closed form of the LOOCV error of augmented RBF models. This result enables WIRBF to adaptively select radial basis functions throughout iterations. Inspired by the bumpiness measure developed by Gutmann (2001), we derive a new pointwise error estimate for RBF predictions using LOOCV. We found out that the inclusion of an unknown point will increase the bumpiness of a RBF interpolation

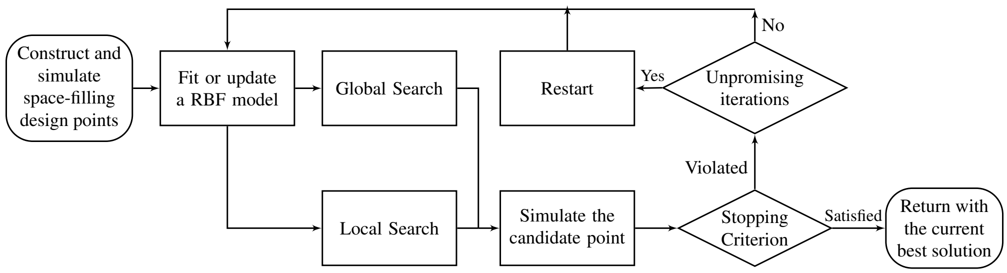

Figure 1: General structure of WIRBF.

model and propose to estimate the increment by LOOCV, which in turn restricts the function value at the unknown point. This error estimate can be efficiently computed and shares several properties with the variance function of kriging models. For example, the prediction error at evaluated points is zero and the prediction error at a unknown point increases with its distance to evaluated points. Based on this new error estimate and the smoothness measure of RBF models, we introduce the weighted improvement to balance the global search and local search with a tunable parameter. Given evaluated points and a target value, the weighted improvement at an unknown point relies on two elements: the improvement and a weight function on each possible improvement. The weight function depends on the smoothness measure that penalizes large deviations from the prediction of the current RBF model. Points with large prediction error and low prediction value show higher weighted improvement. In WIRBF, iterations are declared unpromising when the global RBF model predicts well in the local region. This local prediction accuracy is measured by the local LOOCV that only leave those local points out in the computation.

In the numerical experiments, we consider four alternative approaches EGO (Jones et al. 1998), rbfSolve (Gutmann 2001), MADS-DACE (Audet and Dennis 2006), and MLMSRBF (Regis and Shoemaker 2007). All the five algorithms are compared on 50 test problems, whose dimensions range from 2 to 15 with the median dimension being 8. Data profiles of these algorithms show that WIRBF outperforms existing algorithms. We also find out that LOOCV-based model selection strategy favors MQ for small sample size, while TPS becomes the top choice for a large sample size, and the performance of IMQ, CU and TPS generally increases with the sample size relative to other basis functions.

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