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Approximating Hypervolume Contributions Using Kriging

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ABSTRACT

Hypervolume is an indicator to assess the quality of an obtained solution-set in multi- and many-objective optimization. Hypervolume-based optimization algorithms are rarely used for solving many-objective optimization problems due to the bottleneck of computing the hypervolume contributions of each solution. The current fastest exact hypervolume-computation algorithm is the incremental method [3]. However, it is not scalable to high dimensional problems because the computation cost grows exponentially with respect to problem's dimension. An alternative method for computing hypervolume-contribution is by using approximations, either approximating the total hypervolume or approximating the (least) contributions.

Examples of hypervolume-approximation algorithms have been proposed by Bringmann and Friedrich [5, 4], Ishibuchi, et al. [6], Bader, et al. [1]. Among these algorithms, only [5] has a guaranteed error bound. In this work we propose a novel approximation method, which incorporates uncertainty quantification techniques, based on *kriging* metamodels. Kriging, or Gaussian Process Regression [7], is a metamodeling approach that approximates outputs over the entire search space, and quantifies the uncertainty of the predictor through the mean square error (MSE), also known as *kriging variance* [10]. Kriging is well-known as an effective predictor because the kriging variance can be exploited to control the accuracy of the approximations.

More formally, let $f(\mathbf{x})$ be a deterministic function that is analytically intractable, where $\mathbf{x} = (x_1, ..., x_d)^T$ is an input vector of decision variables of dimension d. In the interest of fitting a kriging metamodel for the response at n design points, kriging assumes that the unknown response surface can be represented as $f(\mathbf{x}) = \mathbf{f}(\mathbf{x})^T\boldsymbol{\beta} + M(\mathbf{x})$, where $\mathbf{f}(\mathbf{x})$ is a vector of known trend functions (i.e., a prior trend model that can be defined as a smoothly varying deterministic function), $\boldsymbol{\beta}$ is a vector of unknown parameters of compatible dimension and $M(\mathbf{x})$ is a realization of a mean zero covariance-stationary Gaussian random field. It is common to consider a constant β instead of the trend term, as it has shown to more useful in practice [8].

In kriging, some samples are taken from the expensive source as training data to build a cheaper prediction model. We consider several metamodels that are fitted with different predictors (e.g., objective values, R2 and crowding distance). The proposed method works as follows: after

computing the e.g. expensive and exact hypervolume contributions of the points in the current front, we fit a kriging metamodel to the response surface of the hypervolume contribution. We exploit the kriging information to search for new points in view of improving the current front. Since for higher dimensions (i.e., more than 10 objectives), even computing the exact hypervolume contribution of each point in the current front is expensive, we also use other indicators with less computational complexity as predictors.

The consistency and correctness rate of the metamodels, as well as the computational cost, are compared against the exact hypervolume contributions and the newly proposed approximation method of Shang, et al.[9]. Preliminary results show that the method has potential. By exploiting both the kriging predictor and its uncertainty, the approximations can be used to sample points in e.g., sequential algorithms such as SMS-EMOA [2], as the computational cost is reduced significantly. Furthermore, we observe that the estimation of the kriging hyperparameters (via maximum likelihood) and the choice of kernel play a crucial role in training the metamodel in order to achieve accurate approximations. Additional experiments will provide valuable information in this regard.

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