

Uncertainty in Surrogate Models

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CCS Concepts

•Computing methodologies → *Continuous space search*;

The existing infill sampling criteria for updating surrogate models come from two objectives: the optimums and the most uncertain points of the surrogate model. The optimums of the surrogate model can improve the exploitation ability of the surrogate model, while most uncertain solutions can help improve the exploration ability by searching the unexplored regions and most efficiently enhancing the accuracy of the surrogate model. It has been shown that the efficiency of surrogate models can be raised if the uncertainty information on the surrogate models is properly used. In this presentation, three points are discussed.

1. Benefits of uncertain solutions to surrogate models: Although uncertainty has been used as an infill sampling criterion, its benefits to surrogate models have not been elaborated in the previous study. Theoretical analysis will be presented.

2. Various ways of measuring uncertainty: There have been different ways to measure the uncertainty. A comprehensive comparison will be given.
3. Uncertainty in ensemble surrogates: Recently, Kriging model became increasingly popular in the field of surrogate-assisted evolutionary algorithms, because it is able to provide a confidence level of the predictions. However, Kriging model has its limitation, which has been largely overlooked. For example, its computational complexity becomes intractable when the number of training samples is large. An alternative to the Kriging model is to use an ensemble consisting of a large number of computationally very efficient models that might provide useful uncertainty information similar to the Kriging model. Empirical results will be shown to verify this idea.

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