Curse and Blessing of Uncertainty in Evolutionary Algorithm Using Approximation

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***Abstract*— Evolutionary frameworks that employ approximation models or surrogates for solving optimization problems with computationally expensive fitness functions may be referred as Surrogate-Assisted Evolutionary Algorithms (SAEA). In this paper, we present a study on the effects of uncertainty in the surrogate on SAEA. In particular, we focus on both the 'curse of uncertainty' and 'blessing of uncertainty' on evolutionary search, a notion borrowed from 'curse and blessing of dimensionality' in [1]. Here, the 'curse of uncertainty' refers to impairments due to the errors in the approximation. The 'blessing of uncertainty' is less explicitly discussed in the literature, but refers to the benefits of approximation errors on evolutionary search. Empirical studies suggest that approximation errors lead to convergence at false global optima, but prove to be beneficial in some cases.**

I. INTRODUCTION

A continuing trend in science and engineering is the use of increasingly accurate simulation codes in the design and analysis process so as to produce ever more reliable and high quality products. Modern Computational Structural Mechanics (CSM), Computational Electro-Magnetics (CEM) and Computational Fluid Dynamics (CFD) analysis represent some of the recent technologies that now play a central role in aiding scientists validate crucial designs and study the effect of altering key design parameters on product performance with astonishingly accuracy. Nonetheless, the use of accurate simulation methods can be very timing consuming, leading to possibly unrealistic design cycle. For example, in a variety of contexts such as drug design, aerospace design, multi-disciplinary structural system, synthesis of proteins in vitro, rainfall prediction, establishing the quality of a potential solution can now take from many minutes to hours or months of supercomputer time. Hence, the overwhelming part of the total run time in such optimization problem is taken up by runs of the computationally expensive simulation codes.

This poses a serious impediment to the practical application of existing optimization algorithms for automatically establishing the critical design parameters present in real world problems in science and engineering. Particularly, modern stochastic optimization methods such as Evolutionary Algorithms (EA) typically require many thousands of function calls to the simulation codes to locate a near optimal solution. It is thus desirable to design novel evolutionary algorithms that are capable of handling optimization problems with computationally expensive fitness function and produce high quality designs under limited computational budgets. Since the design optimization cycle time is directly proportional to the number of calls to the expensive fitness function, in evolutionary search, it is now common practice for computationally cheap approximation models to be used in lieu of exact models to reduce computational cost such as reported in aerodynamic airfoil and aircraft designs in [2], [3], [4], [5].

Specifically, the approximation models are used to replace calls to the computationally expensive codes as often as possible in the evolutionary search process. These approximation models are commonly known as surrogate models or metamodels. Using approximation models, the computational burden can be greatly reduced since the efforts involved in building the surrogate model and optimization using it is much lower than the standard approach of directly coupling the simulation codes with the optimizer. Here, we refer to the class of evolutionary algorithms that employ computationally cheap approximation models to enhance search efficiency as Surrogate-Assisted Evolutionary Algorithms or SAEA in short.

A variety of techniques for the constructions of surrogate model, often also referred to as metamodels or approximation models, have been used in engineering design optimization. Among these techniques, Polynomial Regression (PR, also known as response surface method) [6], [7], Artificial Neural Network (ANN), Radial Basis Function (RBF) [2], [3], [4] and Gaussian Process (GP) (also referred to as Kriging or Design and Analysis of Computer Experiments (DACE) models) [3], [8], [9], [10], [11], are the most prominent and commonly used techniques.

Over the recent years, there have been some notable works on the development of new evolutionary frameworks employing some diverse forms of approximation models. Ratle [8] and El-Beltagy et al. [10] examined strategies for integrating evolutionary search with global surrogate models based on Kriging. Various strategies using GP global surrogate models have also been considered in Ulmer et al. [11] and D. Büche [9]. However, since the idea of constructing accurate global surrogate models might be fundamentally flawed due to the '*curse of dimensionality*', online local surrogate models using RBF was considered in Ong *et al.* [2], Giannakoglou *et al.* [4], Emmerich *et. al.* [12] and Regis *et. al.* [13], in place of global models. Since local

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surrogates are employed, Ong *et al.* [2], also proposed a trust-region memetic approach to interleave use of the exact fitness functions with computationally cheap online RBF local surrogate models. To enhance the approximation accuracy of the surrogates, the framework was subsequently extended to incorporate gradient information [14]. An SAEA based on the combination of a max-min optimization strategy with a Baldwinian trust-region framework employing local surrogate models was also recently proposed in [15] for tackling robust design problems. In contrast to using either global or local surrogate models in most existing SAEA, the synergy between both surrogate models was first investigated for accelerating the convergence of evolutionary search in [3]. Some studies on SAEAs for solving optimization problems with general constraints had also been considered in [2], [12]. In the context of multi-objective evolutionary optimization, the use of approximation models was also recently introduced in Emmerich *et al.* [12], Nain *et al.* [16], Xuan *et al.* [17] and Knowles [18] for solving computational expensive optimization problems. For greater details on some of the strategies typically used in evolutionary computation using approximation models, the reader is referred to the recent survey paper in [19].

In this paper, our focus is to present a study on the effects of uncertainty in the approximated function on SAEA search performance. To date, extensive researches on SAEAs have emphasized on the 'curse of uncertainty', a phrase we use here to refer to the impairment due to the approximation errors of the surrogate model on evolutionary search. In particular, most efforts on designing new SAEA have attempted to do so by focusing on improving the approximation quality of the surrogate model used in the evolutionary search. For instance, most recent SAEA frameworks [2], [3], [8], [12], [13], introduced have generally opted for local over global surrogates which are shown to generate better approximation quality. On the other hand, the 'blessing of uncertainty' which refers to the possible benefits attributed by the approximation errors in the surrogate model on evolutionary search performance, is often neglected. The present work is thus motivated by the lack of study on the impact of uncertainty on SAEA. In particular, the impacts of uncertainty on the Surrogate-Assisted Memetic Algorithm (SAMA) proposed in [2] for solving computationally expensive problems are investigated and discussed in this paper.

The remaining of this paper is organized as follows. In the next section, we briefly outline the proposed SAMA which is used here for investigating the effects of uncertainty in the approximation function on SAEA search performances. In Section III, the impact of uncertainty on the proposed SAMA is illustrated pictorially and discussed conceptually. Empirical studies on commonly used benchmark functions are then conducted to reveal the realistic impact of uncertainty on evolutionary search. The numerical results obtained are then presented and discussed in Section IV while Section V summarizes our main conclusions.

II. Surrogate-Assisted Memetic Algorithm

Here, we consider the general bound constrained nonlinear programming problem of the form:

$$\begin{aligned} \textbf{Minimize}: &\quad f(\mathbf{x}) \\ \textbf{Subject to}: &\quad \mathbf{x}_l \leq \mathbf{x} \leq \mathbf{x}_u, \end{aligned} \tag{1}$$

where $f(\mathbf{x})$ is a scalar-valued objective function, $\mathbf{x} \in \mathbb{R}^d$ is the vector of continuous design variables, and $\mathbf{x}_l$ and $\mathbf{x}_u$ are vectors of lower and upper bounds, respectively. In general SAEA, we are interested in cases where the evaluation of $f(\mathbf{x})$ is computationally expensive, and it is desired to obtain a near optimal solution on a limited computational budget.

Without loss of generality, we consider here the Surrogate-Assisted Memetic Algorithm (SAMA) proposed in [2] for investigating the effects of uncertainty in surrogate function on SAEA. Hence, we briefly outline the SAMA for solving computationally expensive optimization problems in the rest of this section.

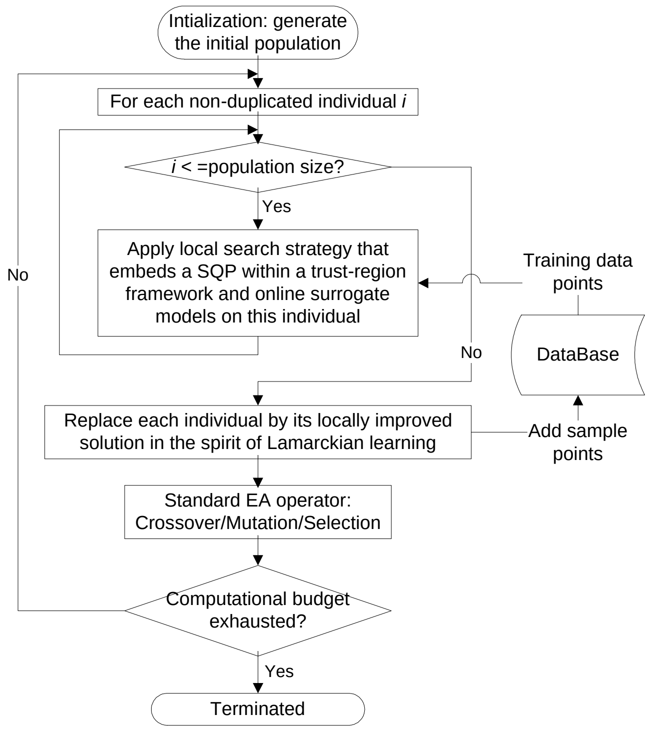

Fig. 1. Flowchart of Surrogate-Assisted Memetic Algorithm

The basic steps of the proposed SAMA optimization framework are depicted in Fig. 1. For the sake of readability, we present the proposed SAMA optimization framework as three main phases:

Phase 1 : At the first step, a population of design points is initialized either randomly or using Design Of Experiments (DOE) techniques such as Latin hypercube sampling [20]. These design points are evaluated using the exact fitness function. The exact fitness values obtained are then archived in a central database together with the design vectors.

Phase 2 : The local search strategy in SAMA embeds a Feasible Sequential Quadratic Programming (FSQP) [21] optimizer within a trust-region framework [22], [23], which ensures convergence to the local optimum of the exact computationally expensive objective function under some mild assumptions. More specifically, for each non-duplicated individuals in the EA population, the local search strategy proceeds with a sequence of trust-region sub-problems of the form:

$$\textbf{Minimize}: \quad \hat{f}^k(\mathbf{x} + \mathbf{x}_c^k) \tag{2}$$

$$\textbf{Subject to}: \quad ||\mathbf{x}|| \leq \Omega^k \tag{3}$$

where $k = 0, 1, 2, \ldots, k_{max}$, $\hat{f}(x)$ is the approximation function corresponding to the objective function $f(x)$. $\mathbf{x}_c^k$ and Ω^k are the starting point and the trust-region radius used for local search at iteration k, respectively.

For each subproblem (or during each trust-region iteration), surrogate models of the exact fitness function, viz., $\hat{f}^k(\mathbf{x})$ are created dynamically. m training data points are extracted from the archived database of design points evaluated so far using the exact analysis codes. These points are then used to construct surrogate models of the exact objective function. Here we consider the use of linear-RBF surrogate model [24], [25], which is constructed by using the m data points in the database chosen strategically based on the individual of interest. In this way, the RBF model offers reasonable accuracy as well as fast training.

Let $\mathcal{D} = \{\mathbf{x}_i, t_i\}, i = 1 \ldots n$ denotes the training dataset, where $\mathbf{x}_i \in \mathbb{R}^d$ and $t_i \in \mathbb{R}$ are the input and output, respectively. Then the surrogate models are interpolating radial basis function networks of the form

$$\hat{f}(\mathbf{x}) = \sum_{i=1}^{n} \alpha_i K(||\mathbf{x} - \mathbf{x}_i||), \tag{4}$$

where $K(||\mathbf{x} - \mathbf{x}_i||) : \mathbb{R}^d \rightarrow \mathbb{R}$ is a radial basis kernel and $\boldsymbol{\alpha} = \{\alpha_1, \alpha_2, \ldots, \alpha_n\} \in \mathbb{R}^n$ denotes the vector of weights.

The surrogate models thus created are used to facilitate the necessary fitness function estimations in the local searches. During local search, we initialize the trust-region Ω using the minimum and maximum values of the design points used to construct the surrogate models. After each iteration, the trust-region radius Ω^k is updated based on a measure which indicates the accuracy of the surrogate model at the kth local optimum, $\mathbf{x}_{lo}^k$. After computing the exact values of the fitness function at this point, the figure of merit, ρ^k, is calculated as

$$\rho^k = \frac{f(\mathbf{x}_c^k) - f(\mathbf{x}_{lo}^k)}{\hat{f}(\mathbf{x}_c^k) - \hat{f}(\mathbf{x}_{lo}^k)}. \tag{5}$$

The above equations provide a measure of the actual versus predicted change in the exact fitness function values at the kth local optimum. The value of ρ^k is then used to update the trust-region radius as follows [22]:

$$\begin{aligned} \Omega^{k+1} &= 0.25\Omega^k, && \text{if } \rho^k \leq 0.25, \\ &= \Omega^k, && \text{if } 0.25 < \rho^k \leq 0.75, \\ &= \xi\Omega^k, && \text{if } \rho^k > 0.75, \end{aligned} \tag{6}$$

where $\xi = 2$, if $||\mathbf{x}_{lo}^k - \mathbf{x}_c^k||_\infty = \Omega^k$ or $\xi = 1$, if $||\mathbf{x}_{lo}^k - \mathbf{x}_c^k||_\infty < \Omega^k$.

The trust-region radius, Ω^k, is reduced if the accuracy of the surrogate, measured by ρ^k is low. Ω^k is doubled if the surrogate is found to be accurate and the kth local optimum, $\mathbf{x}_{lo}^k$, lies on the trust-region bounds. Otherwise the trust-region radius remains unchanged.

The exact solutions of the objective functions at the kth local optimum are combined with the existing neighboring data points to generate new surrogate models in the subsequent trust-region iterations. The initial point for iteration $k+1$ is defined by

$$\begin{aligned} \mathbf{x}_c^{k+1} &= \mathbf{x}_{lo}^k, && \text{if } \rho^k > 0 \\ &= \mathbf{x}_c^k, && \text{if } \rho^k \leq 0. \end{aligned} \tag{7}$$

The trust-region process for an individual terminates when the maximum number of trust-region iterations permissible, k_{max}, chosen by the user, is reached. If an improved solution is found by the local search strategy, the genotype is forced to reflect the result of improvement in the spirit of Lamarckian learning by placing the locally improved individual back into the population to compete for reproductive opportunities.

Phase 3 : The population then proceeds with the standard EA operators of crossover, mutation and selection. This memetic search process is repeated until the computational budget is exhausted or a user specified termination criterion is met.

III. Impact of Uncertainty

In this section, we present the impact of intrinsic approximation errors that exist in the surrogate models on evolutionary search performance. If $f(\mathbf{x})$ denotes the original fitness function and the approximated function is $\hat{f}(\mathbf{x})$, the approximation error at any design point $\mathbf{x}_i$ is $e(\mathbf{x}_i)$, i.e. the uncertainty introduced by the surrogate model at $\mathbf{x}_i$, is then defined as

$$e(\mathbf{x}_i) = |f(\mathbf{x}_i) - \hat{f}(\mathbf{x}_i)| \tag{8}$$

For each non-duplicated individual, if n fitness calls to $\hat{f}(\mathbf{x})$ are made in the SAMA local search strategy, the root mean square error, $rmse$ can be derived as

$$rmse = \sqrt{\frac{\sum_{i=1}^{n} e^2(\mathbf{x}_i)}{n}}. \tag{9}$$

Next, we illustrate the *curse* and *blessing* of uncertainty on SAMA. Without loss of generality, we consider here a minimization problem for $f(\mathbf{x})$.

A. Curse of Uncertainty

The 'curse of uncertainty' is defined here as the impairment due to the approximation errors of the surrogate model on evolutionary search performance. Using the SAMA outlined in Fig 1, we illustrate the possible negative impact of approximation errors on evolutionary search in Fig. 2. The full and dotted line depicted in Fig. 2 denote the original one dimensional function, $f(\mathbf{x})$ and approximated function, $\hat{f}(\mathbf{x})$ assuming only 3 sparse data points, respectively. Note that this is equivalent to using hundreds of data points in multi-variate problems due to the fact that the number of hypercubes required to fill out a compact region of a d-dimensional space grows exponentially with d. Since only three data points are used to approximate the exact fitness function, the approximation quality of the surrogate is expected to be low, i.e., a large $rmse$ is expected.

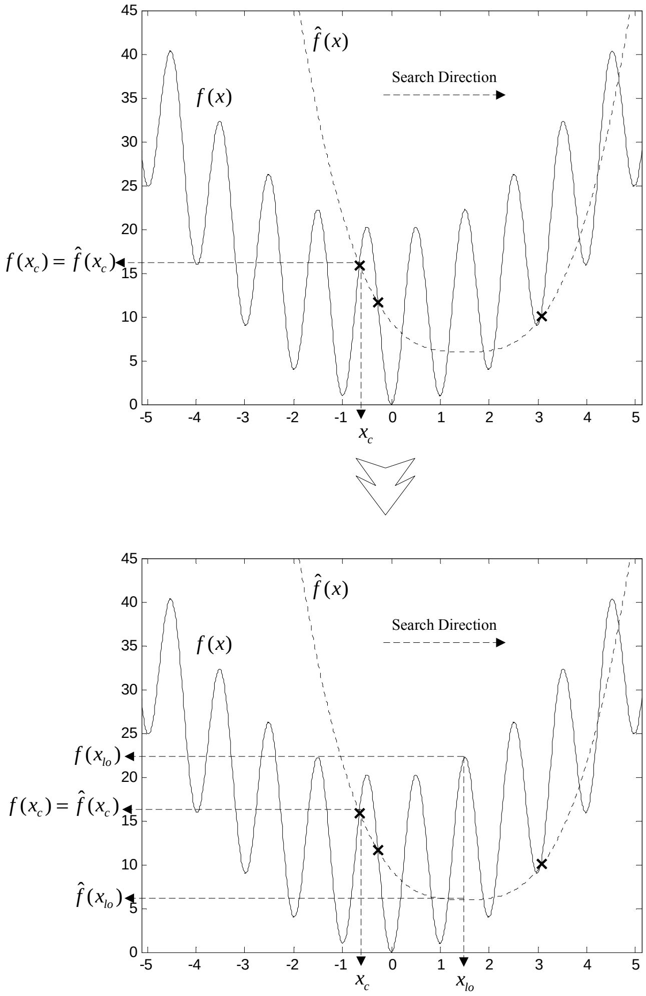

Fig. 2. 'Curse of uncertainty' in Surrogate-Assisted Memetic Algorithm

Assuming that the starting point of the gradient-based local solver in the SAMA is at $\mathbf{x}_c$, where $f(\mathbf{x}_c) = \hat{f}(\mathbf{x}_c)$, the local search is likely to converge to the local optimum of the approximated function situated at $\mathbf{x}_{lo}$ with a predicted fitness value of $\hat{f}(\mathbf{x}_{lo})$ for $k_{max} = 1$. It is worth noting that when $\mathbf{x}_{lo}$ is mapped onto the exact fitness function, it does not provide any fitness improvement over the starting point of $\mathbf{x}_c$ since $f(\mathbf{x}_{lo}) > \hat{f}(\mathbf{x}_{lo})$ and $f(\mathbf{x}_{lo}) > f(\mathbf{x}_c)$.

This explains why extensive research on SAEAs [2], [3], [8], [12], [13], have generally emphasized on improving the accuracy of approximation model as a means to avoid the 'curse of uncertainty' on evolutionary search which is illustrated in Fig. 2.

B. Blessing of Uncertainty

Next we consider the 'blessing of uncertainty', that is less widely discussed, which we use here to refer to the possible benefits attributed by the approximation errors of the surrogate model on optimization search performance.

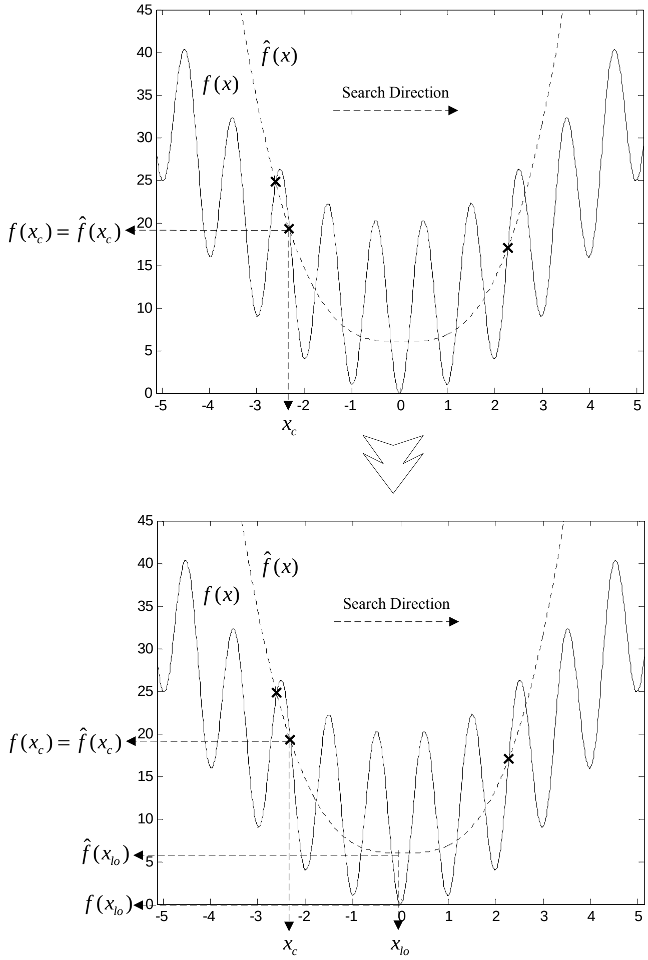

Fig. 3. 'Blessing of uncertainty' in Surrogate-Assisted Memetic Algorithm

In particular, we show that surrogate model with poor approximation accuracy, i.e., having a large $rmse$, can aid the SAMA in accelerating evolutionary search. This is what we referred to the 'blessing of uncertainty' here.

Once again, the full and dotted line in Fig. 3 denote $f(\mathbf{x})$ and $\hat{f}(\mathbf{x})$ assuming 3 other data points, respectively. With the starting point at $\mathbf{x}_c$, it is worth noting that the local search strategy now converges to a local optimum that provides significant fitness improvement over the initial point $\mathbf{x}_c$ with $f(\mathbf{x}_{lo}) < \hat{f}(\mathbf{x}_{lo})$ and $f(\mathbf{x}_{lo}) < f(\mathbf{x}_c)$, thus this type of individual learning accelerates the evolutionary search. Incidentally, $\mathbf{x}_{lo}$ corresponds to the global optimum of the original fitness function. Blessed by the uncertainty or approximation errors in the surrogate model, the SAMA is shown to converge to the global optimum of the original fitness function in a fast track mode.

IV. Empirical Study

In this section, we investigate the impact of uncertainty empirically using the SAMA optimization framework and three commonly used benchmark problems. The results for standard Genetic Algorithm (GA) and Memetic Algorithm (MA) are also reported for comparisons. Note that the MA considered here is a straightforward hybridization between GA and the FSQP local solver. All individuals in the GA undergo culture evolution using the FSQP local solver in the spirit of Lamarckian Learning and no form of approximations is employed. Besides GA and MA, we also consider the SAMA-Perfect in our experimental study. As a control experiment, the SAMA-Perfect is an SAMA that uses the exact fitness function as *zero rmse*, i.e., $rmse = 0$, surrogate models. This implies that the results reported for SAMA-Perfect are obtained in the same manner as the MA. However, in contrast to MA, any exact fitness evaluations incurred during the local search of the MA are disregarded. It is worth noting that SAMA-Perfect is thus considered here to reveal how well an SAEA may perform under perfect approximation quality. As such, any SAMA that performs worse or better than the SAMA-Perfect is clearly attributed to the effect of 'curse of uncertainty' and 'blessing of uncertainty', respectively.

In our experimental study, a standard GA with population size of 50, 1-point crossover and mutation operators at probabilities 0.6 and 0.01, respectively, is employed. A linear ranking selection algorithm is used for selection. However, apart from the standard GA settings, the two user-specified parameters of the SAMA are - 1) number of training data points used to construct the surrogate model m. and 2) maximum trust region iterations k_{max}. In our numerical studies, we set $m = 150$ and $k_{max} = 3$. It should be noted that the m nearest neighbors of the interested individual extracted from the archived database are used to construct the surrogate model here. The criterion used to determine the similarity between design points is the simple Euclidean distance metric.

Three multimodal benchmark problems, i.e., Ackley, Griewank and Rastrigin test functions, are used in the present study since they reflect realistic complex engineering design optimization problems well which are usually multimodal in nature. Figures 4-9 present the search trends of the GA, MA, SAMA and SAMA-Perfect on both the 10D and 20D benchmark functions, i.e., Ackley, Griewank and Rastrigin function. All the benchmark test functions have a single global minimum at $f(\mathbf{x}) = 0.0$ (see the appendix for greater details of the test functions). Note that the results presented are averages of 20 independent runs conducted with a limited computational budget of 6×10^3 exact fitness function evaluations.

From the results of 10D and 20D Ackley, Griewank and Rastrigin test functions depicted in Figures 4-9, it is notable that SAMA and SAMA-Perfect considered here are capable of searching more efficiently than both standard GA and MA on all the benchmark problems under the limited

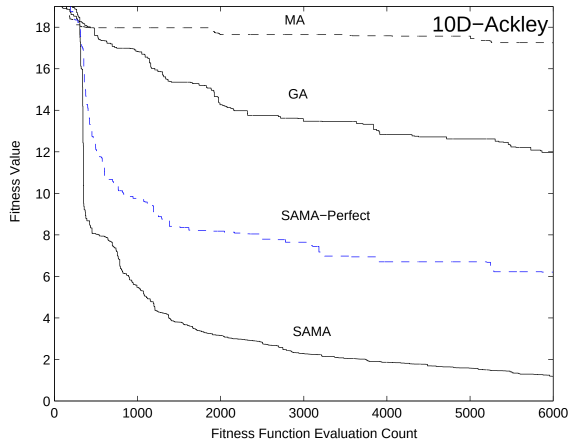

Fig. 4. Convergence trends of the GA, MA, SAMA and SAMA-Perfect framework for 10D Ackley function

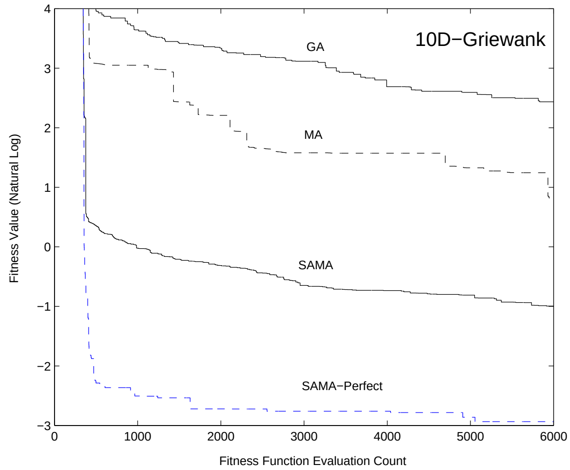

Fig. 5. Convergence trends of the GA, MA, SAMA and SAMA-Perfect framework for 10D Griewank function

computational budget. This makes good sense since memetic algorithms, i.e., EAs that employ local search heavily such as SAMA, are generally well-known to search more efficiently. Further, since the surrogate models are used in place of the exact fitness function when conducting local searches, the SAMA and SAMA-Perfect tend to consume lesser computational efforts than the standard MA for the same search generations. As a result, the SAMA and SAMA-Perfect converges significantly faster than MA.

Most importantly, it is worth highlighting that the SAMA performs significantly better than SAMA-Perfect on both the Ackley and Rastrigin functions (see Fig. 4, 6, 7 and 9). In particular, SAMA converges significantly faster than SAMA-Perfect throughout the entire search on the Ackley test function as depicted in Fig. 4 and 7. This clearly demonstrates the effect of 'blessing of uncertainty' in helping accelerate the evolutionary search. Apparently, the uncertainty or approximation errors in the surrogate model helps in

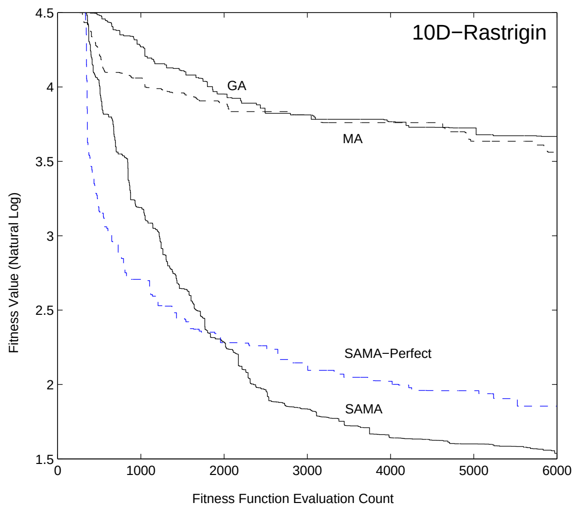

Fig. 6. Convergence trends of the GA, MA, SAMA and SAMA-Perfect framework for 10D Rastrigin function

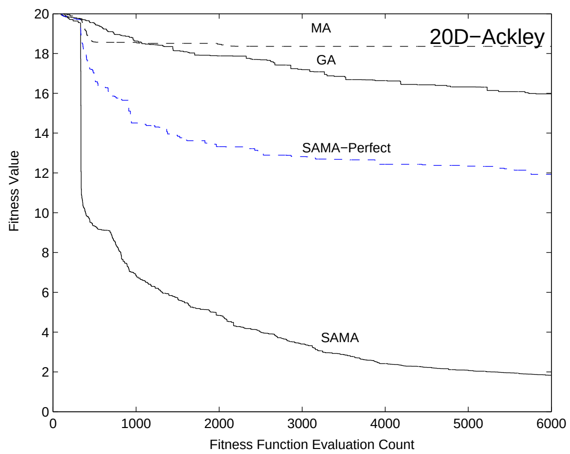

Fig. 7. Convergence trends of the GA, MA, SAMA and SAMA-Perfect framework for 20D Ackley function

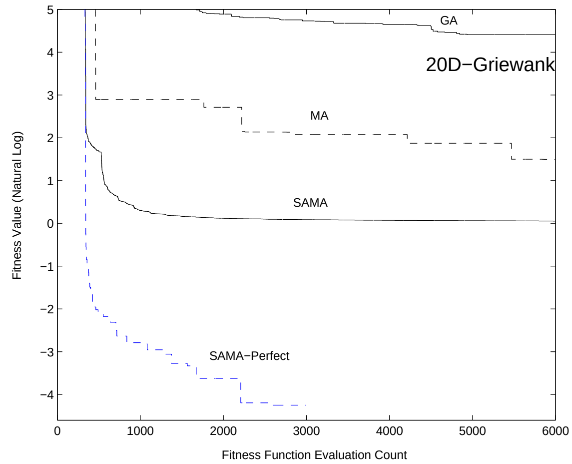

Fig. 8. Convergence trends of the GA, MA, SAMA and SAMA-Perfect framework for 20D Griewank function

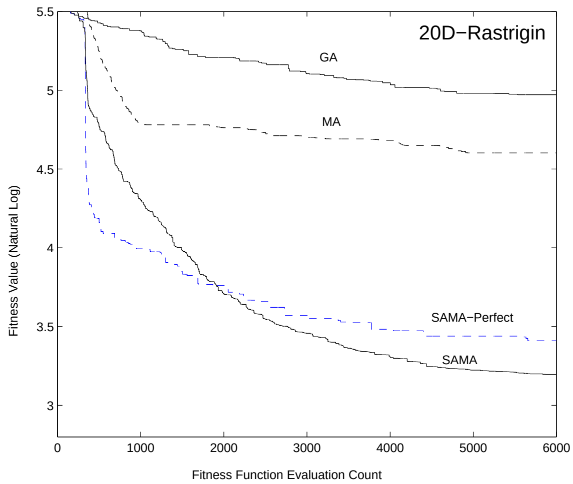

Fig. 9. Convergence trends of the GA, MA, SAMA and SAMA-Perfect framework for 20D Rastrigin function

generalizing or smoothing the multimodal characteristics of the original fitness function, leading to possible super mean convergence rate.

On the other hand, the results in Fig. 5 and 8 suggest that the SAMA-Perfect performs better than SAMA on the Griewank function. Note that this highlights the effect of 'curse of uncertainty' due to the negative impact of approximation errors in the surrogate model which could result the evolutionary search in converging at the false global optima.

In summary, it is worth keeping in mind that the uncertainty introduced by approximation error in the surrogate model is not always bad. In contrast, it may contribute beneficially to the evolutionary search. From the experimental study, the results obtained seem to suggest that it might be more worthwhile to predict search improvement as opposed to the usual practice of improving the quality of the approximation in the context of evolutionary optimization. Essentially, we need a 'paradigm shift' when designing new framework for solving computationally expensive optimization problems with the use of surrogate model. In contrast to existing efforts, it would be more interesting in predicting search improvement in the context of optimization as opposed to the quality of the approximation, which should perhaps be regarded as a secondary objective. In particular, one should concentrate on enhancing optimization search improvements. Besides, mitigating the effect of 'curse of uncertainty', one should also take greater efforts in leveraging from the 'blessing of uncertainty' when designing new SAEA. Hence, one ultimate challenge when designing SAEA is to identify suitable measures of why a surrogate model is good or misleading in predicting search improvements.

As a rule of thumb, one may consider leveraging from the 'blessing of uncertainty' by using more generalized/coarsegrained surrogate models during the early exploration stages of the evolutionary search. Subsequently, higher quality or fine-grained surrogates can be used to avoid getting trapped in any false global optimum when the search reaches the final stages of the evolutionary search.

V. Conclusion

For computationally expensive optimization problems, the use of surrogate models helps to greatly reduce the number of evaluations of the exact fitness function by exploiting the information contained in the search history. In this paper, we have presented the positive and negative impact of the uncertainty introduced by approximation error to evolutionary optimization, otherwise referred to as 'curse of uncertainty' and 'blessing of uncertainty'.

Empirical studies are presented for a number of multimodal benchmark test functions to illustrate the impact of uncertainty using the surrogate-assisted memetic algorithm proposed in [2]. The experimental results are compared with those obtained using a standard GA, MA and SAMA with exact fitness function, i.e., SAMA-Perfect. The results obtained suggest that SAMA is capable of solving computationally expensive optimization problems more efficiently than the standard GA and MA on a limited computational budget. Most importantly, it demonstrates the effect of 'curse of uncertainty' and 'blessing of uncertainty' attributed by approximation errors in the surrogate-assisted evolutionary algorithms, leading to a new paradigm in SAEA design.

VI. Acknowledgment

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Appendix

A. Ackley Test Function

$$20 + e - 20exp(-0.2\sqrt{\frac{1}{n}\sum_{i=1}^{n} x_i^2}) - exp(\frac{1}{n}\sum_{i=1}^{n}\cos 2\pi x_i)$$
$$-32.768 \leq x_i \leq 32.768, i = 1, 2, \ldots, n.$$

B. Griewank Test Function

$$1 + \sum_{i=1}^{n} x_i^2/4000 - \prod_{i=1}^{n}\cos(x_i/\sqrt{i})$$
$$-600 \leq x_i \leq 600, i = 1, 2, \ldots, n.$$

C. Rastrigin Test Function

$$10n + \sum_{i=1}^{n}(x_i^2 - 10\cos(2\pi x_i))$$
$$-5.12 \leq x_i \leq 5.12, i = 1, 2, \ldots, n.$$

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