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Nghia Le Minh, Yew Soon Ong, Stefan Menzel, Yaochu Jin, Bernhard Sendhoff

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Evolution by Adapting Surrogates

Minh Nghia Le mnle@ntu.edu.sg
School of Computer Engineering, Nanyang Technological University, 639798, Singapore

Yew Soon Ong asysong@ntu.edu.sg
School of Computer Engineering, Nanyang Technological University, 639798, Singapore

Stefan Menzel stefan.menzel@honda-ri.de
Honda Research Institute Europe GmbH, 63073 Offenbach/Main, Germany

Yaochu Jin yaochu.jin@surrey.ac.uk
Department of Computing, University of Surrey Guildford, Surrey, GU27XH United Kingdom

Bernhard Sendhoff bernhard.sendhoff@honda-ri.de
Honda Research Institute Europe GmbH, 63073 Offenbach/Main, Germany

Abstract

To deal with complex optimization problems plagued with computationally expensive fitness functions, the use of surrogates to replace the original functions within the evolutionary framework is becoming a common practice. The appropriate data-centric approximation methodology to use for the construction of surrogate model however would depend largely on the nature of the problem of interest, which varies from fitness landscape, state of the evolutionary search to the characteristics of search algorithm used. This has given rise to the plethora of surrogate-assisted evolutionary frameworks proposed in the literature with ad-hoc approximation/surrogate modelling methodologies considered. Since prior knowledge on the suitability of the data-centric approximation methodology to use in surrogate-assisted evolutionary optimization is typically unavailable beforehand, this paper presents a novel evolutionary framework with the *Evolvability Learning* of Surrogates (EvoLS) operating on multiple diverse approximation methodologies in the search. Further, in contrast to the common use of fitness prediction error as criterion for the selection of surrogates, the concept of "*evolvability*" to indicate the productivity or suitability of an approximation methodology that brings about fitness improvement in the evolutionary search is introduced as the basis for adaptation. The backbone of the proposed EvoLS is a statistical learning scheme to determine the *evolvability* of each approximation methodology while the search progresses online. For each individual solution, the most productive approximation methodology is inferred, i.e., the method with highest *evolvability* measure. Fitness improving surrogates are subsequently constructed for use within a trust-region enabled local search strategy, leading to the self-configuration of surrogate-assisted memetic algorithm for solving computationally expensive problems. A numerical study of EvoLS on commonly used benchmark problems and a real-world computationally expensive aerodynamic car rear design problem highlights the efficacy of the proposed EvoLS in attaining reliable, high quality and efficient performance under limited computational budget.

1 Introduction

Engineering reliable and high quality products is now becoming an important practice of many industries to stay competitive in today's increasingly global economy, which is constantly exposed to high commercial pressures. Strong engineering design know-how results in lower time to market and better quality at lower cost. In recent years, advancement in science, engineering and the availability of massive computational power have led to the increasing high-fidelity

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approaches introduced for precise studies of complex systems *in silico*. Modern Computational Structural Mechanics, Computational Electro-Magnetics, Computational Fluid Dynamics and Quantum mechanical calculations represent some of the approaches that have been shown to be highly accurate [Jin, 2002, Zienkiewicz and Taylor, 2006, Hirsch, 2007]. These techniques play a central role in the modelling, simulation and design process since they serve as efficient and convenient alternatives for conducting trials on the original real-world complex system that are otherwise deemed to be too costly or hazardous to construct.

Typically, when high-fidelity analysis codes are used, it is not uncommon for the single simulation process to take minutes, hours to days of supercomputer time to compute. A motivating example at Honda Research Institute is aerodynamic car rear design, where one function evaluation involving a Computational Fluid Dynamics (CFD) simulation to calculate the fitness performance of a potential design can take many hours of wall clock time. Since the design cycle time of a product is directly proportional to the number of calls made to the costly analysis solvers, researchers are now seeking for novel stochastic optimization approaches, including evolutionary frameworks, that handle these forms of problems elegantly. Besides parallelism, which is an obvious choice to achieving near linear order improvement in evolutionary search, researchers are gearing towards surrogate-assisted or meta-model assisted evolutionary frameworks when handling optimization problems imbued with costly non-linear objective and constraint functions [Liang et al., 1999, Jin et al., 2002, Song, 2002, Ong et al., 2003, Jin, 2005a, Lim et al., 2007, Lim et al., 2010, Tenne, 2009, Shi and Rasheed, 2010, Voutchkov and Keane, 2010, Santana-Quintero et al., 2010].

The general consensus on surrogate-assisted evolutionary frameworks is that the efficiency of the search process can be improved by replacing as often as possible, calls to the costly high-fidelity analysis solvers with surrogates that are deemed to be less costly to build and compute. In this manner, the overall computational burden of the evolutionary search can be greatly reduced since the efforts required to build the surrogates and to use them are much lower than those in the traditional approach that directly couples the evolutionary algorithm (EA) with the costly solvers [Serafini, 1998, Booker et al., 1999, Jin et al., 2000, Kim and Cho, 2002, Emmerich et al., 2002, Jin and Sendhoff, 2004, Ulmer et al., 2004, Branke and Schmidt, 2005, Zhou et al., 2005]. Among many data-centric approximation methodologies used to construct surrogates to date, polynomial regression or response surface methodology [Lesh, 1959], support vector machine [Cortes and Vapnik, 1995, Vapnik, 1998], artificial neural networks [Zurada, 1992], radial basis function [Powell, 1987], Gaussian process referred to as Kriging or design and analysis of computer experiment models [Mackay, 1998, Buche et al., 2005] and ensembles of surrogates [Zerpa et al., 2005, Goel et al., 2007, Sanchez et al., 2008, Acar and Rais-Rohani, 2009] are among the most prominently investigated [Jin, 2005a, Zhou et al., 2005, Shi and Rasheed, 2010]. Early proposed approaches have considered using surrogates that target to model the entire solution space or fitness landscape of the costly exact objective or fitness function. However, due to the sparseness of data points collected along the evolutionary search, the construction of accurate global surrogates [Ulmer et al., 2004, Buche et al., 2005] that mimics the entire problem landscape well is impeded by the effect of "curse of dimensionality" [Donoho, 2000]. To enhance the accuracies of the surrogates used, researchers have turned to localized models [Giannakoglou, 2002, Emmerich et al., 2002, Ong et al., 2003, Regis and Shoemaker, 2004] as opposed to globalized models, or their synergies [Zhou et al., 2005, Lim et al., 2010]. Others have also considered the use of gradient information [Ong et al., 2004] to enhance the prediction accuracy of the constructed surrogate models or physics-based models that are deemed to be more trustworthy than pure data-centric counterparts [Keane and Petruzzelli, 2000, Lim et al., 2008].

In the context of surrogate-assisted optimization [Jin et al., 2001, Shi and Rasheed, 2010],

present performance or assessment metrics and schemes used for surrogate model selection and validation involve many prominent approaches that have taken root in the field of statistical and machine learning [Fielding and Bell, 1997, Shi and Rasheed, 2010]. Particularly, the focus have been placed on attaining surrogate model that has minimal apparent error or training error on some optimization data collected during the evolutionary search, as an estimation of the true error when used to replace the original costly high-fidelity analysis solver. Maximum/Mean Absolute Error, Root Mean Square Error (RMSE) and Correlation Measure denote some of the performance metrics that are commonly used [Jin et al., 2001]. Typical model selection schemes that stem from the field of statistical and machine learning, including the split sample (holdout) approach, cross-validation and bootstrapping, are subsequently used to choose surrogate models that have low estimation of apparent and true errors [Queipo et al., 2005, Tenne and Armfield, 2008b]. [Tenne and Armfield, 2008a] used the multiple cross-validation schemes for the selection of low-error surrogates that replace the original costly high-fidelity analysis solver to avoid convergence at false optima of poor accuracy models.

In spite of the significant research effort spent on optimizing computationally expensive problems more efficiently, existing surrogate-assisted evolutionary frameworks may be fundamentally bounded by the use of apparent or training error as the performance metric used to assess and select surrogates. In contrast, it would be more worthwhile to select surrogates that enhance search improvement in the context of optimization, as opposed to the usual practice of choosing surrogate model with minimal estimated true error. Further, the influence of the data-centric approximation methodology employed is deemed to have a major impact on surrogate-assisted evolutionary search performance. The varied suitability of approximation methodology to different fitness landscapes, state of the search, and characteristics of the search algorithm suggests for the varieties of surrogate-assisted evolutionary frameworks in the literature that have emerged with ad-hoc approximation methodology selection. To the best of our knowledge, little work has been done to mitigate this issue since only limited knowledge of the "black-box" optimization problem is available before one starts.

Falling back on the basics of Darwin's grand idea of "Natural Selection" as the criterion for the choice of surrogates that brings about fitness improvement to the search, this paper describes a novel evolutionary search process that evolves along with *fitness improving* surrogates. Here, we focus our study on the *Evolvability Learning* of Surrogates (EvoLS), particularly the adaptive choice of data-centric approximation methodologies that build fitness improving surrogates in place of the original computationally expensive "black-box" problem, during the evolutionary search. In the spirit of reward-based or improvement-based adaptation for the choice of variation operators [Goldberg, 1990, Thierens, 2005, DaCosta et al., 2008], EvoLS infers the fitness improvement contribution of each approximation methodology towards the search, which is here referred to as *evolvability* measure. Hence for each individual or design solution in the evolutionary search, the *evolvability* of each approximation methodology is determined statistically, according to the current state of the search, properties of the search operators and characteristics of the fitness landscape, while the search progresses online. Using the *evolvability* measures derived, the search adapts by using the most productive approximation methodology inferred for the construction of surrogates embedded within a trust-region enabled local search strategy, leading to the self-configuration of surrogate-assisted memetic algorithm that deals with complex optimization of computationally expensive problems more effectively. It is worth noting that to the best of our knowledge, our current effort has not been previously studied in the literature of surrogate-assisted EA.

The paper is outlined as follows: Section 2 introduces the notion of *evolvability* as a performance or assessment measure that expresses the suitability of an approximation methodology in

guiding towards improved evolutionary search and subsequently the essential ingredients of our proposed EvoLS. Section 3 presents a numerical study of EvoLS on commonly used benchmark problems. Detailed analyses on the suitability and cooperation of surrogates in search, as well as the correlation between the estimated *fitness prediction error* and *evolvability* in EvoLS of the surrogate models, are also presented in the section. Section 4 then proceeds to showcase the real world application of EvoLS on an aerodynamic car rear design that involves highly computationally expensive CFD simulations. Finally, Section 5 summarizes the present study with a brief discussion and concludes the paper.

2 Proposed Framework: Evolvability Learning of Surrogates

In this section we present the essential ingredients of the proposed *Evolvability Learning* of Surrogates (EvoLS) for handling computationally expensive optimization problems. In particular, we concentrate on the general nonlinear programming problem of the following form:

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

where $\mathbf{x} \in \mathbb{R}^n$ is the vector of design variables, and $\mathbf{x}_l$, $\mathbf{x}_u$ are vectors of lower and upper bounds, respectively. In this paper, 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, using a novel evolutionary process that adapts fitness improving surrogates, $\widehat{f}_M(\mathbf{x})$ as a replacement of $f(\mathbf{x})$, in the search.

Data-centric surrogates are (statistical) models that are built to approximate computationally expensive simulation codes or the exact fitness evaluations. They are orders of magnitude cheaper to run and can be used in lieu of the exact analysis during evolutionary search. Let $\{(\mathbf{x}_i, t_i)\}_{i=1}^m$ where $t_i = f(\mathbf{x}_i)$ denote the training dataset, where $\mathbf{x} \in \mathbb{R}^n$ is the input vector of scalars or design parameters, and $f(\mathbf{x}) \in \mathbb{R}$ is the output or exact fitness value. Based on the approximation methodology M, the surrogate $\widehat{f}_M(\mathbf{x})$ is constructed as an approximation model of the function $f(\mathbf{x})$. Further, the surrogate model can also yield insights into the functional relationship between the input $\mathbf{x}$ and the objective function $f(\mathbf{x})$.

In what follows, we begin with a formal introduction on the notion of *evolvability* as a performance or assessment measure to indicate the productivity and suitability of an approximation methodology for constructing surrogate that brings about fitness improvement to the evolutionary search (see Section 2.1). The essential backbone of our proposed *Evolvability Learning* of surrogates framework is an evolutionary algorithm coupled with a trust-region enabled local search strategy with adaptive surrogates, in the spirit of Lamarckian learning. In contrast to existing works, we adapt the choice of approximation methodology for the construction of fitness improving data-centric surrogates in place of the original computationally expensive "black-box" problem when conducting the computationally intensive local search in the context of memetic optimization [Hart et al., 2004, Krasnogor and Smith, 2005, Ong et al., 2010] (see Section 2.2).

2.1 Evolvability of Surrogates

Conventionally, surrogate models are assessed and chosen according to their estimated true error, $|f(\mathbf{x}) - \widehat{f}_M(\mathbf{x})|$, where $\widehat{f}_M(\mathbf{x})$ denotes the predicted fitness value of input vector $\mathbf{x}$ by a surrogate constructed using approximation method M. In contrast to existing surrogate-assisted evolutionary search, the surrogate model employed for each individual design solution in the present study favors fitness improvement as the choice of merit to assess the usefulness of surrogates in enhancing search improvement, as opposed to the estimated true error.

In this subsection, we introduce the concept of "*Evolvability*" of an approximation methodology as the basis for adaptation. Since the term "*Evolvability*" has been used in different contexts[1], it is worth highlighting that our concept of *evolvability* generalizes from that of learnability in machine learning [Valiant, 2009]. Here the evolutionary process is regarded as "*evolvable*" on a given optimization problem if the progress in search performance is observed for some moderate number of generations. Hence *evolvability* of an approximation methodology here is referred to the propensity of the method in constructing a surrogate model that guides towards viable, or "potentially favorable" individuals with improved fitness quality.

In particular, the *evolvability* measure of an approximation methodology M for the construction of a fitness improving data-centric surrogate on individual solution $\mathbf{x}$ at generation t, assuming a minimization problem, is denoted here as $Ev_M(\mathbf{x})$ and derived in the form of

$$\begin{aligned} Ev_M(\mathbf{x}) &= Exp[f(\mathbf{x}) - f(\mathbf{y}^{opt})|\mathbf{P}^t, \mathbf{x}] \\ &= f(\mathbf{x}) - \int_y f(\varphi_M(\mathbf{y})) \times P(\mathbf{y}|\mathbf{P}^t, \mathbf{x}) d\mathbf{y} \end{aligned} \tag{1}$$

Here $P(\mathbf{y}|\mathbf{P}^t, \mathbf{x})$ denotes the conditional density function of the stochastic variation operators applied on parent $\mathbf{x}$ to arrive at solution $\mathbf{y}$ at generation t, i.e., $\mathbf{y} \sim P(\mathbf{y}|\mathbf{P}^t, \mathbf{x})$, where $\mathbf{P}^t$ is the current reproduction pool consisting of individual solutions after undergoing natural selection. $\varphi_M(\mathbf{y})$ denotes the resultant solution derived by the local search strategy that operates on the surrogate constructed based on approximation method M. The *evolvability* measure of an approximation methodology indicates the *expectation* of fitness improvement which the refined offspring, denoted here as $\mathbf{y}^{opt} = \varphi_M(\mathbf{y})$, has gained over its parent, upon undergoing local search improvement on the respective constructed surrogate[2]. A high *evolvability* measure encapsulates two core essences of the surrogate-assisted evolutionary search: 1) When a surrogate exhibits low true error estimates, fitness improvement on the refined offspring $\mathbf{y}^{opt}$ over initial parent $\mathbf{x}$ can be expected and 2) When a surrogate exhibits high true error estimates, the discovery of offspring solutions with improved fitness $\mathbf{y}^{opt}$ of $\mathbf{x}$ can be still attained due to the "*blessing of uncertainty*" phenomenon [Ong et al., 2006b] (see Fig. 1 for an example illustration).

Taking into account the current state of the evolutionary search, properties of the search operators, and characteristics of the fitness landscape, a statistical learning approach to estimate the *evolvability* measure $Ev_M(\mathbf{x})$ of each approximation methodology (as defined in Eqn. (1)) for use on a given individual solution $\mathbf{x}$ at generation t, is proposed. Let $\Phi_M = \{(\mathbf{y}_i, \varphi_M(\mathbf{y}_i))\}_{i=1}^K$ denote the database of distinct samples archived along the search, which represents the historical contribution of the approximation methodology on the problem considered. Through a weighted sampling approach, the weight $w_i(\mathbf{x})$ that defines the probability of choosing a sample $(\mathbf{y}_i, \varphi_M(\mathbf{y}_i))$ for the estimation of expected improvement $Ev_M(\mathbf{x})$, or the integral $\int_y f(\varphi_M(\mathbf{y})) \times P(\mathbf{y}|\mathbf{P}^t, \mathbf{x}) d\mathbf{y}$ in particular, is first derived and efficiently estimated here as follows:

$$w_i(\mathbf{x}) = \frac{P(\mathbf{y}_i|\mathbf{P}^t, \mathbf{x})}{\sum_{j=1}^K P(\mathbf{y}_j|\mathbf{P}^t, \mathbf{x})} \tag{2}$$

The weight $w_i(\mathbf{x})$ essentially reflects the current probability of jumping from solution $\mathbf{x}$, via stochastic variation $P(\mathbf{y}|\mathbf{P}^t, \mathbf{x})$, to offspring $\mathbf{y}_i$ which was archived in the database. In

[1] In [Wagner and Altenberg, 1996], "evolvability" is defined as the genome's ability to produce adaptive variants when acted upon by the genetic system. Others have generally referred the term to the ability of stochastic or random variations to produce improvement for adaptation to happen [Ong et al., 2006a].

[2] The local search strategy serves as a function that takes the starting solution $\mathbf{x}$ as input and returns $\mathbf{y}^{opt}$ as the refined solution. As such, the function is represented as $\mathbf{y}^{opt} = \varphi_M(\mathbf{y})$.

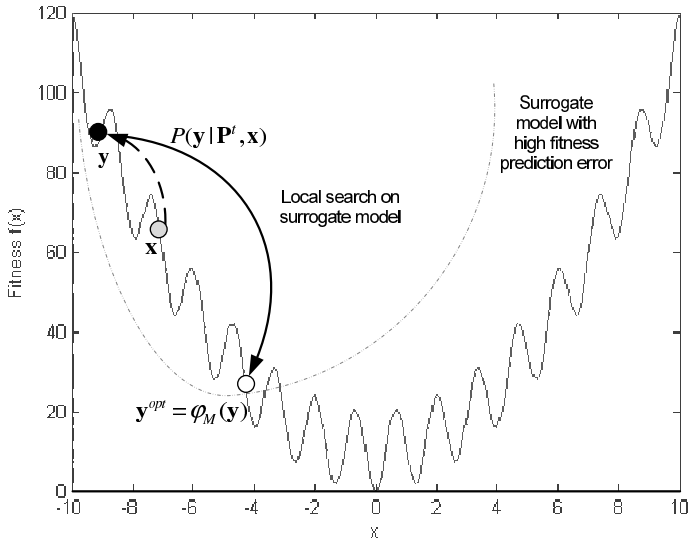


Figure 1: Illustration of *evolvability* under the effect of "*blessing of uncertainty*"

other words, the weight $w_i(\mathbf{x})$ measures the relevancy of the samples $(\mathbf{y}_i, \varphi_M(\mathbf{y}_i))$ for the *evolvability* learning process on solution $\mathbf{x}$. Considering $\{(\mathbf{y}_i, \varphi_M(\mathbf{y}_i))\}_{i=1}^K$ as distinct samples from current distribution $P(\mathbf{y}|\mathbf{P}^t, \mathbf{x})$, the weights $w_i(\mathbf{x})$ associated with samples $(\mathbf{y}_i, \varphi_M(\mathbf{y}_i))$ satisfy the equations: $\sum_{i=1}^K w_i(\mathbf{x}) = 1$ and $w_i(\mathbf{x})$ is proportional to $P(\mathbf{y}_i|\mathbf{P}^t, \mathbf{x})$. Note that the conditional density function $P(\mathbf{y}|\mathbf{P}^t, \mathbf{x})$ is modeled probabilistically based on the properties of the evolutionary variation operators used to reflect the current state of the search. Subsequently, using the archived samples in $\Phi_M = \{(\mathbf{y}_i, \varphi_M(\mathbf{y}_i))\}_{i=1}^K$ and weights w_i obtained using Eqn. (2), $Ev_M(\mathbf{x})$ is estimated as follows:

$$Ev_M(\mathbf{x}) = f(\mathbf{x}) - \sum_{i=1}^{K} f(\varphi_M(\mathbf{y}_i)) \times w_i(\mathbf{x}) \tag{3}$$

2.2 Evolution with Adapting Surrogates

The proposed *Evolvability Learning* of Surrogates (EvoLS) for solving computationally expensive optimization problems is presented and outlined in Algorithm 1. The essential ingredients of our proposed EvoLS framework, are composed of *multiple* data-centric approximation methodologies having diverse characteristics[3], denoted here as $\{M_{id}\}_{id=1}^{ID}$. In the first step, a population of N individuals is initialized either randomly or using design of experiment techniques such as Latin hypercube sampling. The cost or fitness value of each individuals in the population is then determined using $f(\mathbf{x})$. The evaluated population then undergoes natural selection, for instance, via fitness-proportional or tournament selection. Each individual $\mathbf{x}$ in the reproduction pool $\mathbf{P}^t$ is evolved to arrive at the offspring $\mathbf{y}$ using stochastic variation operators including crossover and mutation. Subsequently, with ample design points in the database Ψ or after some predefined database building phase of exact evaluations G_{db} (line 4), the trust-region enabled local search with adaptive surrogate kicks in for each non-duplicated design point or individuals in the population. For a given individual solution $\mathbf{x}$ at generation t, the *evolvability*

[3]Typical approximation techniques are Radial Basic Function (RBF), Kriging or Gaussian process (GP) and Polynomial Regression (PR).

$Ev_{M_{id}}(\mathbf{x})$ of each data-centric approximation methodology is estimated statistically by taking into account the current state of the search, properties of search operators and characteristics of the fitness landscape via the historical contribution by the respective constructed surrogates, while the search progresses online. Without loss of generality, in the event of a minimization problem, the most productive data-centric approximation methodology, which is deemed as one that has the highest estimated *evolvability* measure $\arg\max Ev_{M_{id}}(\mathbf{x})$, is then chosen to construct a surrogate that will be used by the local search to bring about fitness improvement on individual $\mathbf{x}$.

Algorithm 1 Evolvability Learning of Surrogates (EvoLS) Framework

1: *Generate* and *evaluate* an initial population
2: **while** computational budget is not exhausted **do**
3: *Select* individuals for the reproduction pool $\mathbf{P}^t$
4: **if** evaluation count $<$ database building phase (G_{db}) **then**
5: *Evolve* population by evolutionary operators (crossover, mutation)
6: **else**
7: *Evolve* population by evolutionary operators (crossover, mutation)
8: **for** each individual $\mathbf{x}$ in the population **do**
9: *Perform* approximation methodology selection on $\mathbf{x}$ to arrive at M_{id}
10: /*** Local Search Phase on Surrogate Model***/
11: *Find* m nearest points to $\mathbf{y}$ in the database Ψ as training points for surrogate model
12: *Build* surrogate model $\widehat{f}_{M_{id}}(\mathbf{x})$ based on training points
13: *Apply* local search strategy $\varphi_{M_{id}}(\mathbf{y})$ to arrive at $\mathbf{y}_{opt}$
14: *Replace* $\mathbf{y}$ with $\mathbf{y}^{opt}$ (Lamarckian learning)
15: *Archive* sample $(\mathbf{y}, \varphi_{M_{id}}(\mathbf{y}))$ into the database $\Phi_{M_{id}}$
16: **end for**
17: **end if**
18: *Evaluate* new population using exact fitness function $f(\mathbf{x})$
19: *Archive* all exact evaluations $(\mathbf{x}, f(\mathbf{x}))$ into the database Ψ
20: **end while**

The outline of the approximation methodology selection process is detailed in Algorithm 2. It is worth noting on the generality of the proposed framework in the use of density function $P(\mathbf{y}|\mathbf{P}^t, \mathbf{x})$ to represent and reflect the unique characteristics of the stochastic search operators (line 1), thus not restricting to any specific type of operator. By formulating the search operator with a density function, the framework allows the incorporation of different stochastic variation operators, which depends on suitability to the given problem of interest. It is worth highlighting that the condition $\sum_{i=1}^{K} w_i(\mathbf{x}) < \epsilon$ (line 5) caters for the scenario when all samples $(\mathbf{y}_i, \varphi_{M_{id}}(\mathbf{y}_i))$ are irrelevant[4] for evolvability estimation on solution $\mathbf{x}$, i.e., $P(\mathbf{y}_i|\mathbf{P}^t, \mathbf{x})$ is too small. The role of ϵ thus specifies the threshold level of irrelevance for archived samples in the evolvability learning. In particular, ϵ is configured to a precision of $1E-9$ in our present study.

Rather than constructing a global surrogate based on the entire archived samples, nearest sampled points to $\mathbf{y}$ in the database Ψ are selected as training dataset $T = \{(\mathbf{x}_i, f(\mathbf{x}_i))\}_{i=1}^{m}$ for building local fitness improving surrogate $\widehat{f}_{M_{id}}$. The improved solution found using the respective constructed surrogate, denoted here as $\mathbf{y}^{opt} = \varphi_{M_{id}}(\mathbf{y})$, is subsequently evaluated using

[4] At the first generation after the database building phase, note that no data are available for any learning of surrogate evolvability. This case is also considered as "no relevant data available" and the evolvability of surrogate for all methodologies are set to $-\infty$ (line 7, Algorithm 2). In this case, each approximation methodology is randomly selected for use on each individual with the probability of 1/ID (line 13, Algorithm 2).

Algorithm 2 Approximation Methodology Selection Process

Construct density distribution $P(\mathbf{y}|\mathbf{P}^t, \mathbf{x})$ of variation operators
for each approximation methodology M_{id} **do**
  Query archived data $\Phi_{M_{id}} = \{(\mathbf{y}_j, \varphi_{M_{id}}(\mathbf{y}_j))\}$ for M_{id}
  Calculate weight $w_i(\mathbf{x}) = P(\mathbf{y}_i|\mathbf{P}^t, \mathbf{x})$ for each sample $\mathbf{y}_i$
  if $\sum_{i=1}^{K} w_i(\mathbf{x}) < \epsilon$ **then**
    $w_i(\mathbf{x}) = 0$ {No relevant data available}
    $Ev_{M_{id}}(\mathbf{x}) = -\infty$
  else
    $w_i(\mathbf{x}) = w_i(\mathbf{x}) / \sum_{j=1}^{K} w_j(\mathbf{x})$ {Normalize w_i}
    $Ev_{M_{id}}(\mathbf{x}) = f(\mathbf{x}) - \sum_{i=1}^{K} f(\varphi_{M_{id}}(\mathbf{y}_i)) \times w_i(\mathbf{x})$ {Eqn. (3)}
  end if
end for
if $Ev_{M_{id}}(\mathbf{x}) < 0 \; \forall \; M_{id}$ **then**
  Select approximation methodology randomly
else
  Select approximation methodology with highest $Ev_{M_{id}}(\mathbf{x})$ for $\mathbf{x}$
end if

the original computationally expensive fitness function $f(\mathbf{x})$ and replaces the parent individual in the population, in the spirit of Lamarckian learning. Exact evaluations of all newly found individuals $\{(\mathbf{y}^{opt}, f(\mathbf{y}^{opt}))\}$, together with $\{(\mathbf{y}, \varphi_{M_{id}}(\mathbf{y}))\}$ are then archived into the database Ψ and $\Phi_{M_{id}}$, respectively, for subsequent use in the search. The entire process repeats until the specified stopping criteria are satisfied.

3 Empirical Study

In this section, we present the numerical results obtained by the proposed EvoLS using three commonly used approximation methodologies, namely: 1) interpolating linear spline Radial Basic Function (RBF), 2) 2nd order Polynomial Regression (PR) and 3) interpolating Kriging/ Gaussian Process (GP). For the details on GP, PR and RBF, the reader is referred to Section 5. Representative *30* dimensional benchmark problems considered in the present study are summarized in Table 1 while the algorithmic parameters of EvoLS are summarized in Table 2.

The stochastic variation operators considered in the present study are uniform crossover and mutation, which have been widely used in real-coded genetic evolution. For the sake of brevity, we consider the use of simple variation operators in our illustrating example to showcase the mechanism and generality of the proposed EvoLS. It is worth noting that other advanced real-parameter search operators, such as that discussed in [Herrera et al., 1998], can also be considered in the framework through density distribution $P(\mathbf{y}|\mathbf{P}^t, \mathbf{x})$.

In particular, the crossover procedure considered here is outlined as follows: a) randomly select two solutions, $\mathbf{x}$ and $\mathbf{x}'$ from the population; b) perform uniform crossover on $\mathbf{x}$ and $\mathbf{x}'$ to create two offspring $\mathbf{y}_1$ and $\mathbf{y}_2$ where the locus i of offspring $\mathbf{y}_1^{(i)}/\mathbf{y}_2^{(i)}$ has value $\mathbf{x}_1^{(i)}/\mathbf{x}_2^{(i)}$ with crossover probability of p_{cross}, and c) select $\mathbf{y} = \mathbf{y}_1$ or $\mathbf{y}_2$ as the offspring of $\mathbf{x}$. Uniform mutation is conducted on $\mathbf{y}$ such that each locus $\mathbf{y}^{(i)}$ is assigned to a random value bounded by $[\min_{j=1\ldots N}\{\mathbf{x}_j^{(i)}\}, \max_{j=1\ldots N}\{\mathbf{x}_j^{(i)}\}]$ with a mutation probability of p_{mut}. Note that N denotes the population size.

The task of deriving exact density distribution function is non-trivial due to the complexity of the search dynamics. Thus a simplified assumption of uniformity in the offspring distribution

Table 1: Benchmark problems considered in the empirical study. On shifted rotated problems, note that $\mathbf{z} = \mathbf{M} \times (\mathbf{x} - \mathbf{o})$ where $\mathbf{M}$ is the rotation matrix and $\mathbf{o}$ is the shifted global optimum. Otherwise, $\mathbf{z} = \mathbf{x}$.

Function	Benchmark test functions	Range of x	Multi*	Non-sep*
Ackley (F1)	$F_{Ackley} = 20 + e - 20e^{-0.2\sqrt{\frac{1}{n}\sum_{i=1}^{n} z_i^2}} - e^{\frac{1}{n}\sum_{i=1}^{n}\cos(2\pi z_i)}$	$[-32, 32]^n$	Yes	Yes
Griewank (F2)	$F_{Griewank} = 1 + \sum_{i=1}^{n} z_i^2/4000 - \prod_{i=1}^{n}\cos(z_i/\sqrt{i})$	$[-600, 600]^n$	Yes	Yes
Rosenbrock (F3)	$F_{Rosenbrock} = \sum_{i=1}^{n-1}(100 \times (z_{i+1} - z_i^2)^2 + (1 - z_i)^2)$	$[-2.048, 2.048]^n$	Yes	Yes
Shifted rotated Rastrigin (F4)	$F_{Rastrigin-SR} = 10n + \sum_{i=1}^{n}(z_i^2 - 10\cos(2\pi z_i))$	$[-5, 5]^n$	Yes	Yes
Shifted rotated Weierstrass (F5)	$F_{Weierstrass-SR} = \sum_{i=1}^{n}(\sum_{k=0}^{k_{max}}(a^k \cos(2\pi b^k(z_i + 0.5)))) - n\sum_{k=0}^{k_{max}}(a^k \cos(\pi b^k))$	$[-0.5, 0.5]^n$	Yes	Yes
Expanded Griewank plus Rosenbrock (F6)	$F_{Grie+Rosen} = \sum_{i=1}^{D} F_{Griewank}(F_{Rosenbrock}(z_i, z_{i+1}))$ $z_{D+1} = z_1$	$[-3, 1]^n$	Yes	Yes

is considered for practical purposes in our empirical study. The density distribution $P(\mathbf{y}|\mathbf{P}^t, \mathbf{x})$ is then modeled as a uniform distribution with

$$P(\mathbf{y}|\mathbf{P}^t, \mathbf{x}) = UniformDist(\mathbf{R}) = \begin{cases} \frac{1}{Vol(\mathbf{R})} & \textit{if } \mathbf{y} \in \mathbf{R} \\ 0 & \textit{otherwise} \end{cases} \quad (4)$$

where $Vol(\mathbf{R})$ denotes the hyper-volume of hyper-rectangle with bounds $\mathbf{R}$ defined as

$$\mathbf{R} = [\min_{j=1\ldots N}\{\mathbf{x}_j^{(i)}\}, \max_{j=1\ldots N}\{\mathbf{x}_j^{(i)}\}]_{i=1\ldots n}$$

Note that the stochastic variations considered impose the resultant offspring $\mathbf{y}$ to be bounded by $\min_{j=1\ldots N}\{\mathbf{x}_j^{(i)}\}$ and $\max_{j=1\ldots N}\{\mathbf{x}_j^{(i)}\}$ for each dimension[5], i.e., $\forall i = 1\ldots n$. Since the hyper-rectangle $\mathbf{R}$ reduces as the search progresses, the probabilistic model of the variation operators reflects well on the refinement of the search space throughout the evolution.

On the other hand, the local search strategy of EvoLS involves a trust-region framework [Ong et al., 2006b] with Broyden-Fletcher-Goldfarb-Shanno (L-BFGS-B) method [Zhu et al., 1997]. Note that under mild assumptions, trust-region framework ensures theoretical convergence to the local optimum or stationary point of the exact objective function, despite the use of surrogate models [Alexandrov et al., 1998, Ong et al., 2003]. For each individual $\mathbf{y}_i$ in the population, the local search method L-BFGS-B proceeds on the inferred most productive surrogate model $\widehat{f}_M(\mathbf{x})$ to perform a sequence of trust-region sub-problems of the form:

$$\begin{aligned} \textbf{Minimize}: \quad & \widehat{f}_M(\mathbf{y} + \mathbf{y}_i^k) \\ \textbf{Subject to}: \quad & ||\mathbf{y}|| \leq \Omega^k \end{aligned}$$

[5] If $\mathbf{x}_1$, $\mathbf{x}_2$ and $\mathbf{y}$ denote the parents and offspring, then each locus of the offspring $\mathbf{y}$ satisfies the inequality

$$\min\{\mathbf{x}_1^{(i)}, \mathbf{x}_2^{(i)}\} \leq \mathbf{y}^{(i)} \leq \max\{\mathbf{x}_1^{(i)}, \mathbf{x}_2^{(i)}\}, \forall i = 1\ldots n \quad (5)$$

where $k = 0, 1, 2, \ldots k_{max}$, $\widehat{f}_M(\mathbf{y})$ denotes the approximate function corresponding to the original fitness function $f(\mathbf{y})$, $\mathbf{y}_i^k$ and Ω^k denote the starting point and trust-region radius at iteration k, respectively. For each individual $\mathbf{y}_i$, the surrogate model $\widehat{f}_M(\mathbf{y})$ of the original fitness function is created dynamically using training data from archived database $\Psi = \{(\mathbf{x}_i, f(\mathbf{x}_i))\}_{i=1}^{Q}$ to estimate the fitness during local search. Note that $\mathbf{y}_i^{k+1} = \arg\min \widehat{f}_M(\mathbf{y} + \mathbf{y}_i^k)$ denotes the local optimum of the trust-region sub-problem at iteration k. At each kth iteration, $\mathbf{y}_i^{k+1}$ and the trust-region radius Ω^k are updated accordingly. In the present study, the resultant individual denoted here as $\mathbf{y}_i^{k_{max}} = \varphi_M(\mathbf{y}_i)$, is the improved solution attained by L-BFGS-B over surrogate model $\widehat{f}_M(\mathbf{x})$.

Table 2: Algorithm Configuration

Parameters	
Population size	100
Selection scheme	Roulette wheel
Stopping criteria	8000 evaluations
Local search method	L-BFGS-B
Number of trust region iteration	3
Crossover probability (p_{cross})	1
Mutation probability (p_{mut})	0.01
Variation operator	Uniform crossover and mutation
Database building phase (G_{db})	2000 evaluations
Precision Accuracy	1E-8

3.1 Search Quality and Efficiency of EvoLS

To see how adapting the choice of most productive approximation methodology affects the performance and efficiency of the search as compared to the use of single approximation method, in this subsection, the performance of Symbiotic Evolution is compared with the canonical surrogate-assisted evolutionary algorithms (SAEAs) with single approximation methodology, i.e., EA-RBF, EA-PR and EA-GP. Note that the procedure of canonical SAEA is consistent to the EvoLS outlined in Algorithm 1, except that the former lacks any approximation methodology selection mechanism (line 11). In addition, EA-Perfect, which refers to a canonical SAEA that employs an imaginary approximation method that generates error-free surrogates [6] is also considered here to assess the benefits of using *evolvability* measure versus approximation errors as the criterion for model selection.

The averaged convergence trends obtained by EvoLS on the benchmark problems as a function of the total number of exact fitness function evaluations are summarized in Figs. 2(a)-2(f). The results presented here are the average of 20 independent runs for each test problem. Also shown in the figures are the averaged convergence trends obtained using the canonical surrogate-assisted evolutionary algorithms (SAEAs), i.e., EA-RBF, EA-PR, EA-GP and EA-Perfect. Using the statistical non-parametric Wilcoxon test at 95% confidence level, the search performances of EvoLS when pitted against each SAEA considered on solving the set of benchmark problems, are then tabulated in Table 3. To facilitate a fair comparison study, the parametric configurations of EvoLS and SAEAs are maintained consistent, as defined in Table 2. The detailed numerical results of the algorithms considered in the study are summarized in Table 5.

[6] An error-free surrogate model is realized by using exact fitness function for evaluation inside the local search strategy where a surrogate model should be used. Note that the incurred fitness evaluation here is not counted as part of the computational budget.

Table 3: Results of Wilcoxon test at 95% confidence level, for EvoLS and other SAEAs in solving the 30D benchmark problems. Note that s+, s- or $\approx$ indicates that EvoLS is significantly statistically better, worse or indifferent, respectively.

Algorithm	EA-GP	EA-PR	EA-RBF	EA-Perfect
F_{Ackley}	s+	$\approx$	s+	s+
$F_{Griewank}$	s+	s-	s+	s-
$F_{Rosenbrock}$	s-	s+	s+	s-
$F_{Rastrigin-SR}$	s+	s+	s+	s+
$F_{Weiertrass-SR}$	s+	$\approx$	s+	s+
$F_{Grie+Rosen}$	s+	s+	$\approx$	s+

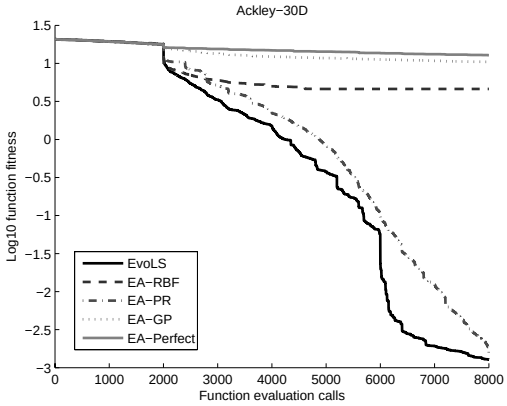
Statistical analysis shows that EvoLS fares competitively or significantly outperforms most of the methods considered, at 95% confidence level on the 30-dimensional benchmark problems. In the ideal case of error-free surrogate model, denoted by EA-Perfect, the results indicated that the search on surrogate model with low approximation error does not always lead to better performance over the others. As one would expect, the EA-Perfect exhibits superior performance on the low-modality Rosenbrock (with 2 local optima [Shang and Qiu, 2006]) and Griewank (which has a relatively smooth fitness landscape at high dimensionalities [Le et al., 2009]), as observed in Figs. 2(b)-2(c), due to the high efficacy of the local search strategy used on a *perfect* or error-free model. However, on problems with highly multi-modal and rugged landscapes including Ackley, Rastrigin-SR, Weierstrass-SR and expanded Griewank plus Rosenbrock (see Figs. 2(a), 2(d)-2(f)), EvoLS which operates on inferring the most suitable approximation method according to their *evolvability* measure, is observed to outperform EA-Perfect significantly.

Focusing on the Griewank function, it is worth noting that EvoLS exhibits more robust search than EA-PR, as indicated by the relatively lower standard deviation in solution quality (as shown in Table 5). Similar robustness in the EvoLS over EA-GP can also be observed on the Rosenbrock function. On the other hand, the competitive performance displayed by EA-PR and EvoLS on 3 out of the 6 benchmark problems suggests both are benefitting well from the landscape smoothing effect of low-order polynomial regression. Such a phenomenon is established as the "*blessing of uncertainty*" in SAEA [Lim et al., 2010]. Overall, the results from the statistical tests confirmed the robustness and superiority of the EvoLS over those that assumed a single fixed approximation methodology throughout the search (EA-GP, EA-PR, EA-RBF and EA-Perfect).

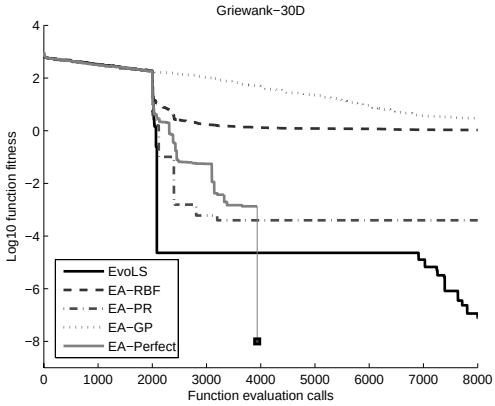
In Table 4, the percentage of savings in computational budget by EvoLS (in terms of the number of calls made to the original computational expensive function) to arrive at equivalent solution quality to the respective algorithms on the 30D benchmark problems, are tabulated. Note that only those algorithms that are significantly outperformed by EvoLS on the respective benchmark problem are discussed here. The superior efficiency of the EvoLS over the counterpart algorithms can be observed from the table, where significant savings of 25.32% to 74.91% are noted.

3.2 Suitability of Surrogates

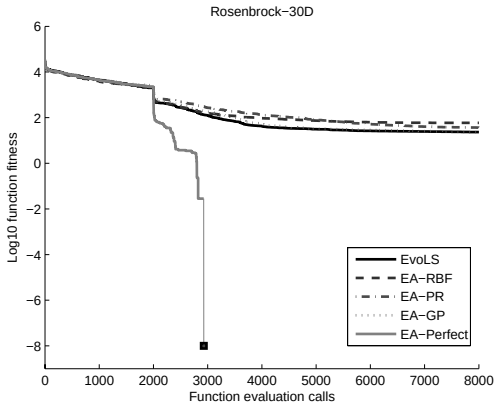
In this subsection, the suitability of surrogates in evolutionary search with respect to the benchmark problem of interest, prediction quality and states of the evolution are investigated and discussed.



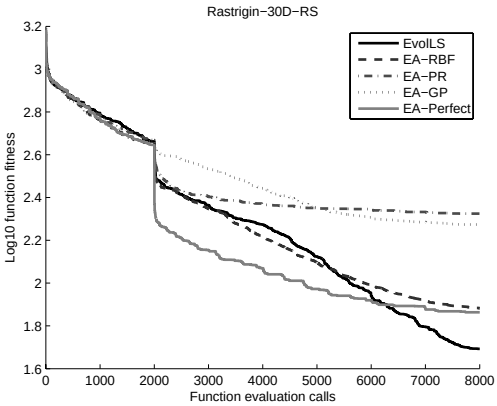
(a) **Ackley-30D**



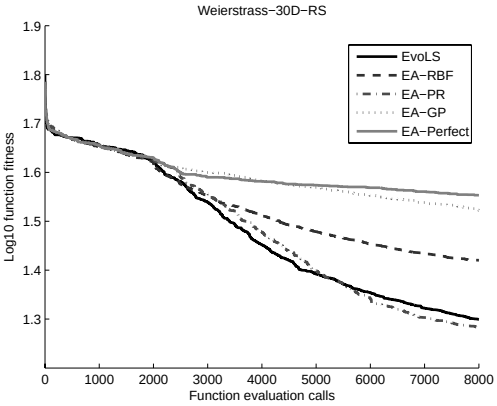
(b) **Griewank-30D**



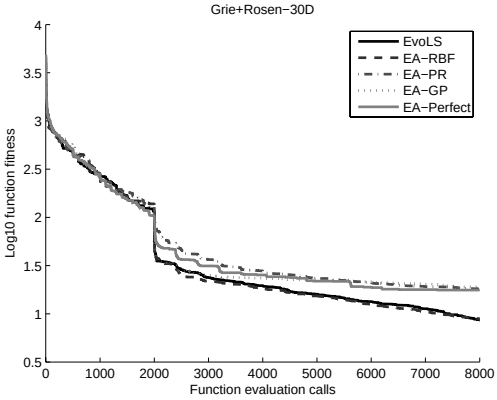
(c) **Rosenbrock-30D**



(d) **Rastrigin-30D-RS**



(e) **Weierstrass-30D-RS**



(f) **Grie+Rosen-30D**

Figure 2: Performance of EvoLS and SAEAs on the benchmark problems. Note that the average fitness values are plotted in logarithmic scale to highlight the differences in the search performances.

Table 4: Percentage of savings in computational budget by EvoLS on the benchmark problems, in terms of the number of calls made to the original computational expensive function to arrive at equivalent converged solution quality of the respective algorithms.

Algorithm	EA-GP	EA-PR	EA-RBF	EA-Perfect
F_{Ackley}	74.60	-	66.91	74.91
$F_{Griewank}$	74.76	71.75	74.76	-
$F_{Rosenbrock}$	-	50.27	55.20	-
$F_{Rastrigin-SR}$	49.64	55.31	26.33	25.32
$F_{Weiertrass-SR}$	58.57	-	42.28	63.32
$F_{Grie+Rosen}$	47.67	45.05	-	44.13

3.2.1 Fitness Landscapes

The summarized search performances of the algorithms with single approximation methodology (i.e., RBF, PR or GP), as tabulated in Table 5, confirm our hypothesis that the suitability of surrogates in an evolutionary search largely depends on problem fitness landscape. For the purpose of our discussion here, we focus the attention on the results for EA-PR and EA-RBF. EA-PR is observed to outperform other SAEAs with single approximation method (GP or RBF) on Ackley and Griewank, while EA-RBF emerging as superior on Rastrigin-SR and expanded Griewank plus Rosenbrock. Through adapting the choice of suitable approximation methodology by means of *evolvability* learning while the search progresses online, EvoLS is noted to attain search performances that are better or at least competitive to the best performing SAEA (with single approximation method) for the respective problems considered.

3.2.2 Prediction Quality and Fitness Improving Surrogate

In this subsection, we discussed the correlations between prediction quality and surrogate suitability in bringing about the search improvement in EvoLS. The correlations can be assessed by analyzing the average frequency of usage and the normalized root mean square fitness prediction errors (N-RMSE) of the surrogates (or the associated approximation methodology used to construct the surrogate), across the search[7], such as that depicted in Figs. 3(a) and 3(b), respectively. From Fig. 3, it is notable that the low-error fitness prediction surrogates constructed using RBF have been beneficial in enhancing the search towards the refinement of solutions with improved fitness. The presence of fitness improving surrogates thus naturally led to the high frequency of usage of RBF in EvoLS . Conversely, negative correlations between fitness prediction quality and surrogate suitability may also occur to benefit search. Here, we illustrate one such scenario observed in our study. In spite of the high-error fitness predictions exhibited by the 2nd-order polynomial regression (PR) on Griewank (as can be observed in Fig. 3), the persistently high frequency of usage for PR in EvoLS clearly depicts the inference towards productive fitness improving over fitness error-free surrogates.

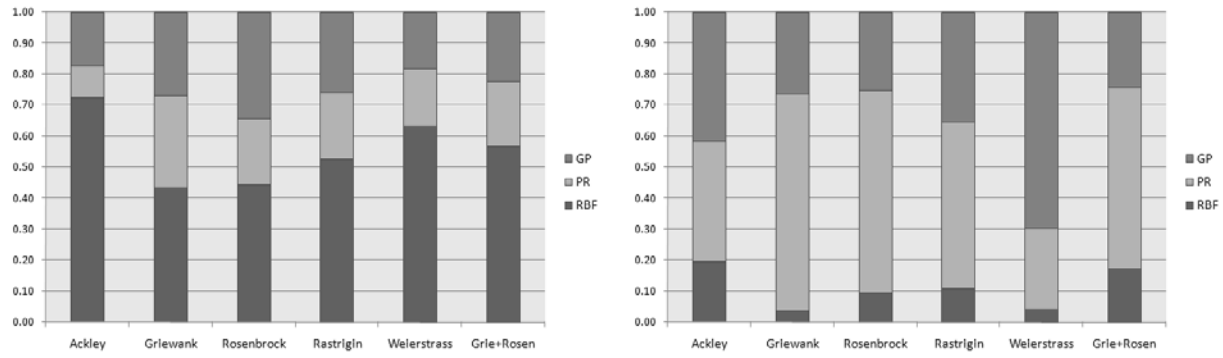
3.2.3 State of Evolution

To assess the suitability of the surrogates at different stages of the evolution, next we analyze the fitness prediction errors of the surrogates and their frequencies of usage in the EvoLS search, which are summarized in Figs. 4(a)-4(f). The upper subplot of each figure depicts how often

[7] For each generation t, the root mean square (RMS) prediction errors of all methodologies (GP, PR and RBF) are first computed across the independent runs and subsequently normalized, thus bringing the prediction errors to the common scale of [0, 1] throughout the different stages of the search. Subsequently, for each problem, the normalized RMSEs of GP, PR and RBF are averaged across all generations of the entire search.

Table 5: Statistics of the converged solution quality at the end of 8000 exact function evaluations for EA-GP, EA-PR, EA-RBF and EvoLS on benchmark problems.

Optimization	**Ackley (F1)**				
Algorithm	Mean	Std. Dev.	Median	Best	Worst
EA-GP	1.05E+01	4.42E+00	1.23E+01	1.17E-03	1.53E+01
EA-PR	1.54E-03	8.34E-04	1.30E-03	4.93E-04	3.39E-03
EA-RBF	4.62E+00	1.67E+00	4.47E+00	2.66E+00	6.40E+00
EA-Perfect	1.28E+01	1.17E+00	1.30E+01	9.73E+00	1.42E+01
EvoLS	1.28E-03	9.84E-04	1.13E-03	1.32E-04	3.40E-03
Optimization	**Griewank (F2)**				
Algorithm	Mean	Std. Dev.	Median	Best	Worst
EA-GP	2.67E+00	1.12E+01	1.88E-02	4.02E-05	5.02E+01
EA-PR	3.96E-04	1.27E-03	3.77E-09	4.34E-10	5.04E-03
EA-RBF	1.07E+00	3.03E-01	1.10E+00	2.43E-01	1.47E+00
EA-Perfect	6.02E-019	1.51E-019	5.96E-019	3.25E-019	8.67E-019
EvoLS	7.89E-08	2.80E-07	1.12E-08	1.71E-09	1.17E-06
Optimization	**Rosenbrock (F3)**				
Algorithm	Mean	Std. Dev.	Median	Best	Worst
EA-GP	2.29E+01	1.76E+01	1.92E+01	1.47E+01	9.70E+01
EA-PR	3.63E+01	2.29E+01	2.81E+01	2.66E+01	1.18E+02
EA-RBF	5.90E+01	2.15E+01	5.57E+01	3.07E+01	1.02E+02
EA-Perfect	5.65E-18	2.04E-17	1.05E-18	2.96E-019	9.22E-17
EvoLS	2.32E+01	1.66E+00	2.29E+01	2.11E+01	2.66E+01
Optimization	**Shifted Rotated Rastrigin (F4)**				
Algorithm	Mean	Std. Dev.	Median	Best	Worst
EA-GP	1.88E+02	7.42E+01	1.79E+02	6.67E+01	3.44E+02
EA-PR	2.11E+02	1.36E+01	2.12E+02	1.86E+02	2.39E+02
EA-RBF	7.63E+01	2.86E+01	8.02E+01	3.43E+01	1.38E+02
EA-Perfect	7.30E+01	1.54E+01	6.99E+01	4.97E+01	1.09E+02
EvoLS	4.93E+01	1.66E+01	4.73E+01	2.36E+01	8.16E+01
Optimization	**Shifted Rotated Weierstrass (F5)**				
Algorithm	Mean	Std. Dev.	Median	Best	Worst
EA-GP	3.33E+01	4.42E+00	3.42E+01	2.44E+01	3.99E+01
EA-PR	1.91E+01	2.61E+00	1.93E+01	1.38E+01	2.37E+01
EA-RBF	2.63E+01	2.97E+00	2.63E+01	2.08E+01	3.29E+01
EA-Perfect	3.57E+01	2.64E+00	3.58E+01	3.15E+01	4.12E+01
EvoLS	1.99E+01	2.69E+00	1.97E+01	1.52E+01	2.52E+01
Optimization	**Expanded Griewank plus Rosenbrock (F6)**				
Algorithm	Mean	Std. Dev.	Median	Best	Worst
EA-GP	1.90E+01	4.58E+00	1.87E+01	1.20E+01	2.81E+01
EA-PR	1.81E+01	1.04E+00	1.81E+01	1.61E+01	2.04E+01
EA-RBF	8.85E+00	2.03E+00	9.25E+00	5.84E+00	1.17E+01
EA-Perfect	1.76E+01	6.26E+00	1.66E+01	9.27E+00	3.67E+01
EvoLS	8.60E+00	1.78E+00	8.77E+00	6.27E+00	1.15E+01



(a) **Frequency** of usage of surrogate models.

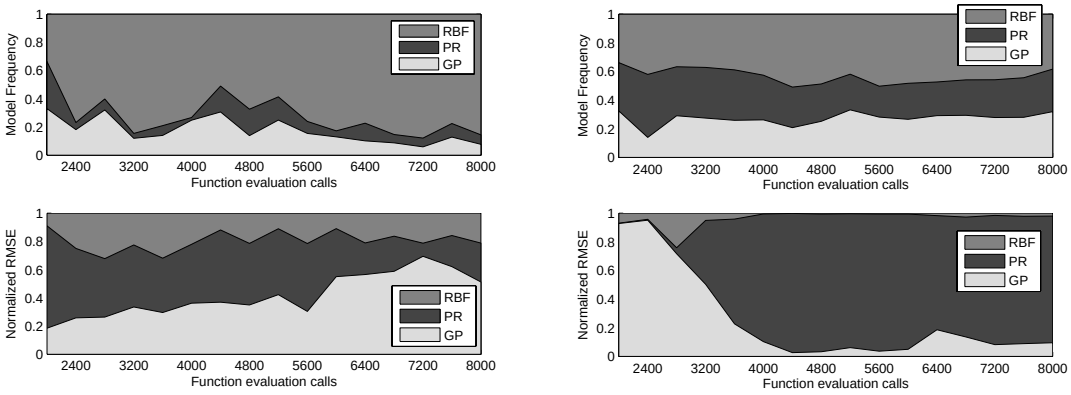
(b) **Fitness prediction error** of surrogate models.

Figure 3: Correlation analyses of EvoLS on the benchmark problems

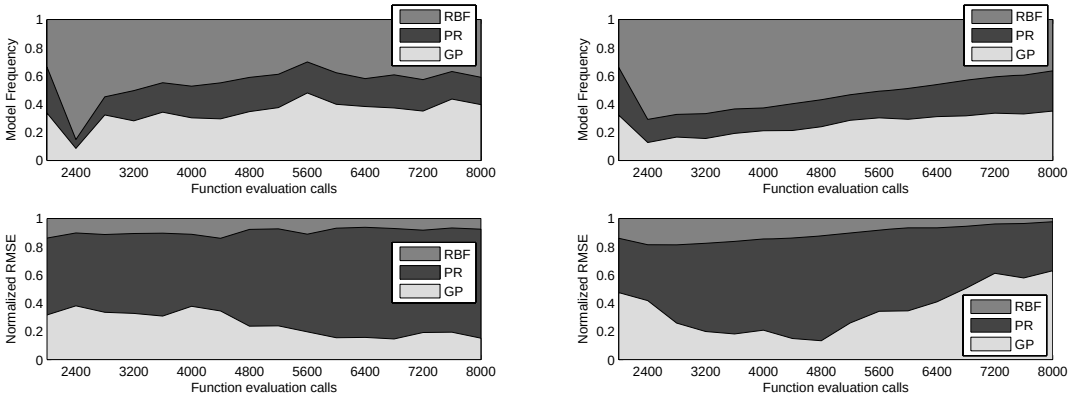
an approximation methodology is inferred as most productive and hence chosen for use within the local search strategy of the EvoLS. The lower subplot, on the other hand, depicts the root mean square fitness prediction errors of the respective surrogates. The results from Fig. 4 suggest that no single approximation methodology has served as most suitable throughout the different stages of the search. For instance, RBF is noted to be used more prominently than the other approximation methodologies at the initial stages of the search but then exhibits a decreasing trend in frequency of usage at the later stage of the search on both the Rosenbrock and rotated shifted Rastrigin (see Figs. 4(c), 4(d)). Likewise, the fitness prediction qualities of GP is noted to be significantly low at the initial stage of the search on Griewank (see Fig. 4(b)) but the error eases as the search evolves. Note that such variations in fitness prediction qualities of the PR model can also be observed on Ackley (see Fig. 4(a)). These results in a way strengthens our aspiration towards the notion of evolvability and hence the significance of EvoLS in facilitating productive cooperation among diverse approximation methodologies, working together to accomplish the shared goal of effective and efficient global optimization in the evolutionary search.

3.3 Assessment Against Other Surrogate-assisted and Evolutionary Search Approaches

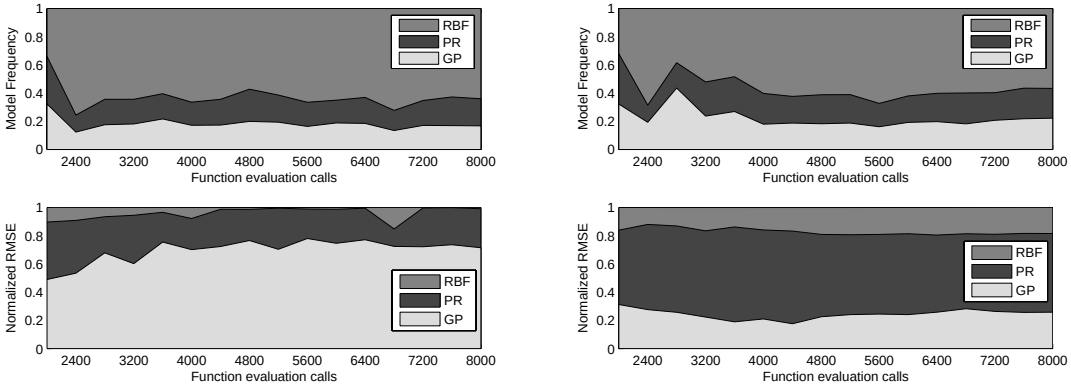
In this section, we further assess the proposed EvoLS against other recent state-of-the-art evolutionary approaches reported in the literature. In particular, GS-SOMA [Lim et al., 2010] and IPOP-CMA-ES [Auger and Hansen, 2005], which are well established evolutionary algorithms designed for numerical optimization under the scenarios of limited computational budget, are included here as the state-of-the-art algorithms for comparison. Using a statistical Wilcoxon test at 95% confidence level, the search performances of each algorithms are pitted against the EvoLS on solving the set of benchmark functions described in Table 1, where the results are tabulated in Table 6. Note that all algorithms considered are configured to their default parametric settings in [Lim et al., 2010, Auger and Hansen, 2005] to facilitate a fair comparison in our study. The detailed statistics of the algorithms from 20 independent runs on the numerical errors with respect to the global optimum are provided separately in Table 7. From the statistical results in Table 6, EvoLS is observed to fare competitively or significantly outperforms the state-of-the-art methods GS-SOMA and IPOP-CMA-ES, at 95% confidence level on the 30-dimensional benchmark problems, thus highlighting the robustness and superiority of EvoLS.



(a) **Ackley-30D** (b) **Griewank-30D**



(c) **Rosenbrock-30D** (d) **Rastrigin-30D-RS**



(e) **Weierstrass-30D-RS** (f) **Grie+Rosen-30D**

Figure 4: Surrogate Frequencies of Usage and Fitness Prediction Errors in EvoLS Search

Table 6: Results of Wilcoxon test at 95% confidence level for EvoLS, GS-SOMA and IPOP-CMA-ES in solving the 30D benchmark problems. Note that s+, s- or $\approx$ indicates that EvoLS is significantly statistically better, worse or indifferent, respectively.

Algorithm	GS-SOMA	IPOP-CMA-ES
F_{Ackley}	s+	s+
$F_{Griewank}$	s+	s+
$F_{Rosenbrock}$	s+	s+
$F_{Rastrigin-SR}$	s+	$\approx$
$F_{Weiertrass-SR}$	s+	s+
$F_{Grie+Rosen}$	s+	$\approx$

Table 7: Statistics of the converged solution quality at the end of 8000 exact function evaluations for GS-SOMA, IPOP-CMA-ES and EvoLS on benchmark problems.

Optimization	**Ackley (F1)**				
Algorithm	Mean	Std. Dev.	Median	Best	Worst
GS-SOMA	3.58E+00	5.09E-01	3.67E+00	2.87E+00	4.28E+00
IPOP-CMA-ES	5.89E+00	9.24E+00	9.67E-04	4.14E-08	2.03E+01
EvoLS	7.43E-05	9.16E-05	4.22E-05	7.48E-06	3.71E-04
Optimization	**Griewank (F2)**				
Algorithm	Mean	Std. Dev.	Median	Best	Worst
GS-SOMA	2.20E-03	4.60E-03	8.95E-09	1.40E-10	1.54E-02
IPOP-CMA-ES	1.97E-03	5.45E-03	4.09E-11	5.73E-12	2.22E-02
EvoLS	1.38E-13	6.17E-13	1.12E-16	1.08E-19	2.76E-12
Optimization	**Rosenbrock (F3)**				
Algorithm	Mean	Std. Dev.	Median	Best	Worst
GS-SOMA	4.63e+01	2.92e+01	3.02e+01	2.83e+01	1.26e+02
IPOP-CMA-ES	2.24E+01	1.82E+00	2.21E+01	1.98E+01	2.63E+01
EvoLS	2.01E+01	1.71E+00	2.00E+01	1.71E+01	2.31E+01
Optimization	**Shifted Rotated Rastrigin (F4)**				
Algorithm	Mean	Std. Dev.	Median	Best	Worst
GS-SOMA	2.04E+02	1.60E+01	2.07E+02	1.66E+02	2.30E+02
IPOP-CMA-ES	6.11E+01	4.16E+01	5.11E+01	3.28E+01	2.31E+02
EvoLS	4.72E+01	1.79E+01	4.75E+01	2.36E+01	7.48E+01
Optimization	**Shifted Rotated Weierstrass (F5)**				
Algorithm	Mean	Std. Dev.	Median	Best	Worst
GS-SOMA	2.60E+01	3.05E+00	2.90E+01	2.40E+01	3.40E+01
IPOP-CMA-ES	2.22E+01	2.62E+00	2.24E+01	1.70E+01	2.95E+01
EvoLS	1.96E+01	2.14E+00	1.97E+01	1.52E+01	2.27E+01
Optimization	**Expanded Griewank plus Rosenbrock (F6)**				
Algorithm	Mean	Std. Dev.	Median	Best	Worst
GS-SOMA	1.80E+01	1.05E+00	1.77E+01	1.70E+01	1.90E+01
IPOP-CMA-ES	3.42E+00	6.27E-01	3.44E+00	1.93E+00	4.70E+00
EvoLS	3.34E+00	4.32E-01	3.41E+00	2.46E+00	4.09E+00

4 Real-World Application: Aerodynamic Optimization of the Rear of a Car Model

Our ultimate motivation of the present work lies in the difficulties and challenges posed by computationally expensive real-world applications. In this section, we consider the proposed EvoLS for the design of a quasi-realistic aerodynamic car rear using a simplified model version of the Honda Civic. The objective is to minimize the aerodynamic performance calculation of the design, i.e., the total drag of the car rear. The design model of the Honda Civic used in the present study is labelled here as *Baseline-C-Model*. Aerodynamic car rear design is an extremely complex task that is normally undertaken over an extended time period and at different levels of complexity. In this application, an aerodynamic performance calculation of the design requires a Computational Fluid Dynamics (CFD) simulation that generally takes around 60 minutes wall-clock time on a Quad-Core machine. For the calculation, the *OpenFOAM* CFD flow solver [Jasak et al., 2007, Jasak and Rusche, 2009] used allows a tight integration into the optimization process, providing an automatic meshing procedure as well as parallelization.

The choice of an adequate geometrical representation of the car simulation model that can be reasonably coupled to the optimization algorithm is also crucial. In the presented experiments, the state-of-the-art *Free Form Deformation* (FFD) [Sederberg and Parry, 1986, Coquillart, 1990] has been chosen as the geometrical representations since it provides a fair trade-off between design flexibility and scalable number of optimization parameters. FFD is a shape morphing technique that allows smooth design changes using an arbitrary number of parameters which are intuitively adjustable to the problem at hand. The benefits of FFD can be found in [Menzel and Sendhoff, 2008].

For the technical realization, the application of FFD requires a control volume, i.e. a lattice of control points, in which the model geometry is embedded. In the next step the geometry is transferred to the spline parameter space of the control volume, a numerical process which is called "freezing". After the object is frozen it is possible to select and move single or several control points to generate deformed shape variations. To amplify the surface deformations, it is important to position the control points close to the car body. Fig. 5 illustrates the *Baseline-C-Model* as well as the implemented FFD control volume. Based on this set-up, ten optimization parameters p_i have been chosen. Each parameter comprises a group of 22 control points within one layer of the control volume as marked by the dashed box in the lower left image of Fig. 5. Since the model is symmetric to the center plane in y-direction, the parameters affect the left and right side of the car in the same way.

During the evaluation step of the optimization process, the aerodynamic performance of each design solution, i.e. the total drag of the car, is calculated. Therefore, each of the ten parameters stored in the design solution or individual are extracted and added as an offset on the corresponding layer of control points, either in x-direction $(p_1, p_3, p_5, p_7, p_9)$ or in z-direction $(p_2, p_4, p_6, p_8, p_{10})$. Second, based on the modified control points, the car shape is updated using FFD and stored as a triangulated mesh, i.e. STL file format. Third, the external air flow around the car is computed by the *OpenFOAM* CFD solver. Therefore, a CFD calculation grid around the updated car shape has to be generated and is automatically carried out using the *snappyHexMesh* tool of *OpenFOAM*. Based on this grid, the external air flow is calculated, resulting in a drag value that is monitored every 10th time step of the simulation. After the calculation has sufficiently converged, the total drag value is extracted and assigned to the individual.

4.1 Fitness Landscape Analysis

To conduct a preliminary analysis on the conditions of the problem fitness landscape, the effect of design variables on drag at the car rear is investigated in this section. In particular, 700 samples of design solutions generated randomly using the Latin hypercube sampling technique

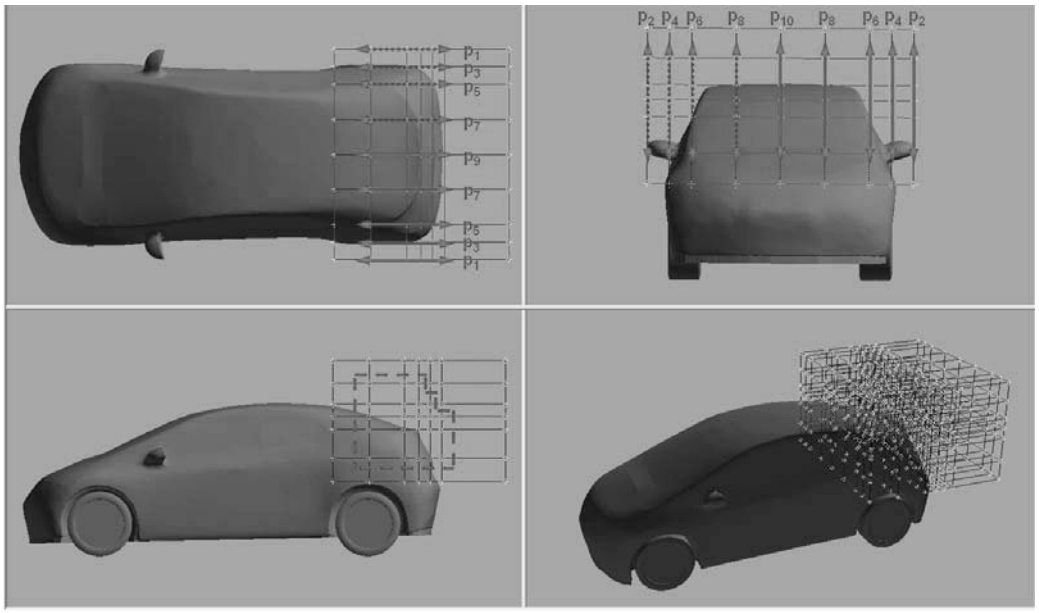


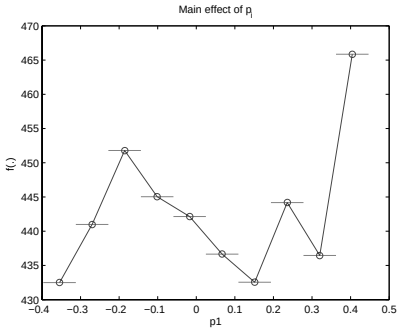
Figure 5: Experiment Set-up

and the corresponding aerodynamic performance (i.e., total drag) from the SimpleBase-C-Model landscape are first grouped into different bins for each dimension (variable). The average fitness of each bin is plotted against the control variable for the sensitivity analysis.

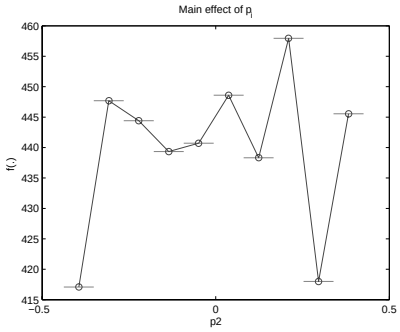
The plots for samples drawn from the search range of $[-0.4, 0.4]$, divided into 10 bins, are presented in Fig. 6. The significantly non-monotonic trends in each subplot of the design variables, especially in Figs. 6(a), 6(b), 6(c), 6(f) and 6(j), indicate the existence of multiple minima/maxima in the search space, thus illustrating the multi-modal and rugged fitness landscape of the quasi-realistic aerodynamic car rear design problem.

4.2 Optimization Results

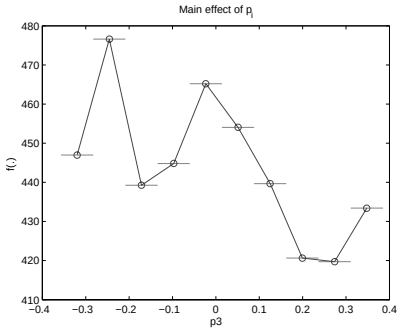
Due to the highly computationally expensive CFD simulations, a computational budget of 200 exact evaluations (200 hours) is used for one optimization run in our study. A small population size of 10 was considered in EvoLS. Note that no database building phase (i.e., $G_{db} = 0$) is required by EvoLS in this case since sufficient sample data of the search space was available at hand. The convergence trend of the best run for the aerodynamic car rear design problem obtained by EvoLS (as described in Section 3) after 200 evaluations on the aerodynamic car rear design problem is shown in Fig. 7. The optimization results obtained previously based on the Covariance Matrix Adaptation Evolution Strategy [Hansen and Kern, 2004], including CMA-ES(5, 10) and CMA-ES(1, 10), are also reported in the figure for comparison. As shown in the figure, due to the complexity of the problem landscape, CMA-ES(1, 10) as an individual-based search strategy performed worst as compared to the other population-based approaches. Among the algorithms considered, EvoLS exhibited the best performances by locating the car rear design with the lowest drag value of $\mathbf{403.573}$. The search trends also show that the proposed EvoLS arrived at the best design solution discovered by CMA-ES(5, 10) using only $1/2$ of the computational budget incurred by the latter. The computational saving of more than 50% and improved solution quality attained thus show that in a practical setting the usage of the proposed



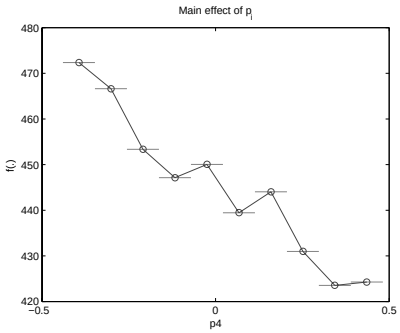
(a) **Main effect of** p_1



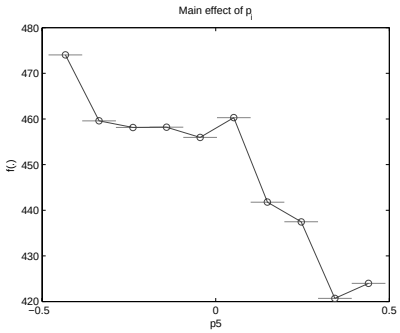
(b) **Main effect of** p_2



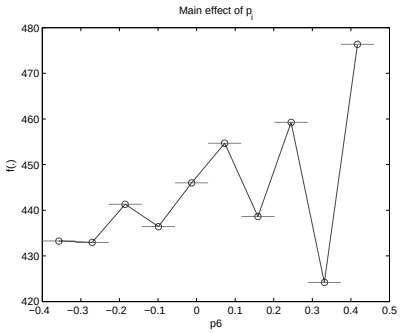
(c) **Main effect of** p_3



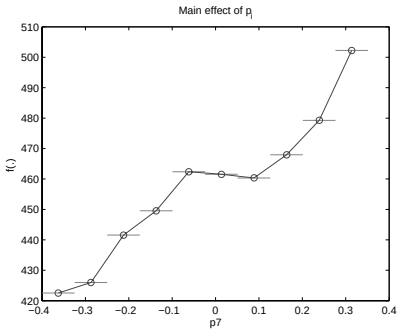
(d) **Main effect of** p_4



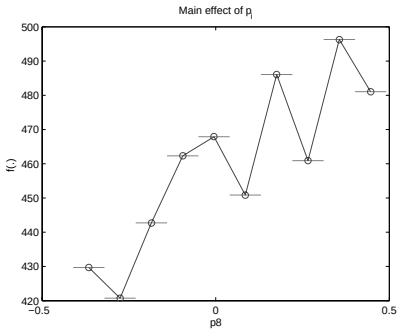
(e) **Main effect of** p_5



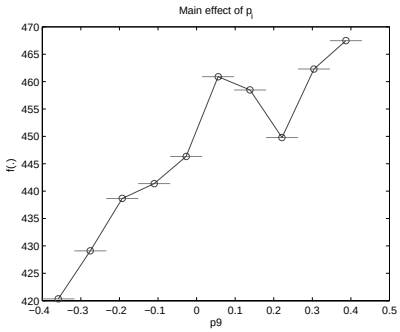
(f) **Main effect of** p_6



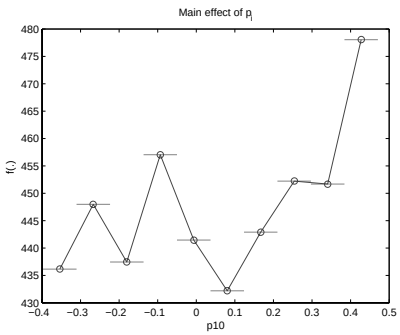
(g) **Main effect of** p_7



(h) **Main effect of** p_8



(i) **Main effect of** p_9



(j) **Main effect of** p_{10}

Figure 6: Landscape Analysis of the Aerodynamic Car Rear Design Problem

EvoLS can be highly beneficial as compared to standard techniques for solving challenging computationally expensive design optimization.

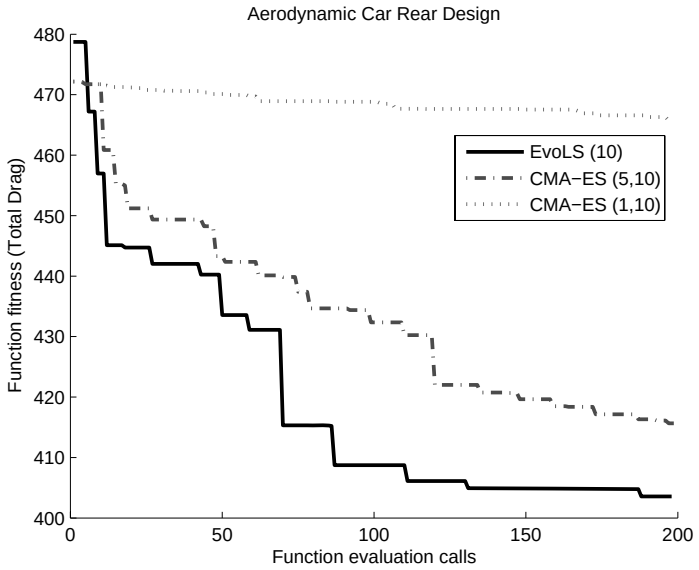


Figure 7: Convergence Trace on Aerodynamic Car Rear Design

5 Conclusions

In this article, we have presented a novel *Evolvability Learning* of Surrogates (EvoLS) framework that operates on *multiple* approximation methodologies of diverse characteristics. The suitability of an approximation method in the construction of surrogates for guiding the search is assessed by the *evolvability* metric instead of solely focusing on the fitness prediction error. By constructing the respective surrogate using the most productive approximation method inferred for each individual solution in the population, EvoLS serves as a self-configurable surrogate-assisted memetic algorithm for optimizing computationally expensive problems at improved search performance.

Numerical study of EvoLS with assessment made against the use of single approximation methodology or the imaginary perfect surrogates as well as other state-of-the-art algorithms on commonly used benchmark problems demonstrated the robustness and efficiency of EvoLS. Further analysis on the suitability of surrogates operating within EvoLS also confirmed our motivations to introduce the evolvability measure that takes into account the current state of the search, properties of the search operators and characteristics of the fitness landscape, while the search progress online. EvoLS thus serves as a novel effort towards the design of frameworks that promote competition and cooperation among diverse approximation methodologies, working together to accomplish the shared goal of global optimization in the evolutionary search. Last but not least, the results on the real-world computationally expensive problem of aerodynamic car rear design further highlighted the competitiveness of EvoLS in attaining improved search performance.

Appendix A: Surrogate Modelling

There exist a variety of approximation methodologies for constructing surrogate models that take its roots from the field of statistical and machine learning field [Jin, 2005b, Shi and Rasheed, 2010]. One popular approach in the design optimization literature is polynomial regression or response surface methodology [Lesh, 1959]. Neural networks which have shown to be effective tools for function approximation have also been employed as surrogates extensively in evolutionary optimization. These include support vector machine [Cortes and Vapnik, 1995, Vapnik, 1998], artificial neural networks [Zurada, 1992] and radial basis function [Powell, 1987]. A statistically sound alternative is Gaussian process or Kriging [Mackay, 1998], referred to as design and analysis of computer experiment models. Next, we provide a brief overview on three different approximation methods used in the paper, namely, polynomial regression (PR), radial basic function (RBF) and Gaussian process (GP).

Polynomial Regression

The most widely used polynomial regression model is the quadratic model which takes the form

$$\widehat{f}_M(\mathbf{x}) = \beta_0 + \sum_{i=1}^{n} \beta_i \mathbf{x}^{(i)} + \sum_{1 \le i \le j \le n} \beta_{n-1+i+j} \mathbf{x}^{(i)} \mathbf{x}^{(j)} \tag{6}$$

where n is the number of input variables, $\mathbf{x}^{(i)}$ is the i-th component of $\mathbf{x}$, and β_i are the coefficients to be estimated. As the number of terms in the quadratic model is $n_t = (n+1)(n+2)/2$ in total, the number of training sample points should be at least n_t for proper estimation of the unknown coefficients, by means of either least square or gradient-based methods [Jin, 2005a].

Radial Basic Function

The surrogate models in this category are interpolating radial basic function (RBF) networks of the form

$$\widehat{f}_M(\mathbf{x}) = \sum_{i=1}^{m} \alpha_i K(\| \mathbf{x} - \mathbf{x}_i \|) \tag{7}$$

where $K(\| \mathbf{x} - \mathbf{x}_i \|) : \mathbb{R}^d \to \mathbb{R}$ is a RBF and $\boldsymbol{\alpha} = [\alpha_1, \alpha_2, \ldots, \alpha_m]^T \in \mathbb{R}^m$ denotes the vector of weights. The number of hidden nodes used in interpolating RBF is often assumed as equal to the number of training vector points.

Typical choices for the kernel function include linear splines, cubic splines, multiquadrics, thin-plate splines and Gaussian functions [Bishop, 1996]. Given a suitable kernel, the weight vector $\boldsymbol{\alpha}$ can be computed by solving the linear algebraic system of equations

$$\mathbf{K}\boldsymbol{\alpha} = \mathbf{t}$$

where $\mathbf{t} = [t_1, t_2, \ldots, t_m]^T \in \mathbb{R}^m$ denotes the vector of outputs and $\mathbf{K} \in \mathbb{R}^{m \times m}$ denotes the Gram matrix formed using the training inputs (i.e., the *ij*-th element of $\mathbf{K}$ is computed as $K(\| \mathbf{x}_i - \mathbf{x}_j \|)$).

Kriging/Gaussian Process

The Kriging model or Gaussian Process (GP) assumes the presence of a global model $g(\mathbf{x})$ and an additive noise term $Z(\mathbf{x})$ in the original function.

$$f(\mathbf{x}) = g(\mathbf{x}) + Z(\mathbf{x})$$

where $g(\mathbf{x})$ is a known function of $\mathbf{x}$ as a global model of the original function, and $Z(\mathbf{x})$ is a Gaussian random function with zero mean and non-zero covariance that represents a localized

noise or deviation from the global model. Usually, $g(\mathbf{x})$ is a polynomial and in many cases, it is reduced to a constant β. The approximation model of $f(\mathbf{x})$, given the m samples and the current input $\mathbf{x}$, is defined as:

$$\widehat{f}_M(\mathbf{x}) = \widehat{\beta} + \mathbf{r}^T(\mathbf{x})\mathbf{R}^{-1}(\mathbf{t} - \widehat{\beta}\mathbf{I}) \tag{8}$$

where $\mathbf{t} = [t_1, t_2, \ldots, t_m]^T$, $\mathbf{I}$ is a unit vector of length m, and $\mathbf{R}$ is the correlation matrix which can be obtained by computing the correlation function between any two samples, i.e., $\mathbf{R}_{i,j} = R(\mathbf{x}_i, \mathbf{x}_j)$. While the correlation function can be specified by the user, Gaussian exponential correlation function, defined by correlation parameters $\{\theta_k\}_{k=1}^n$, has often been used:

$$R(\mathbf{x}_i, \mathbf{x}_j) = \exp\left[-\sum_{k=1}^{n} \theta_k |\mathbf{x}_i^{(k)} - \mathbf{x}_j^{(k)}|^2\right]$$

where $\mathbf{x}_i^{(k)}$ and $\mathbf{x}_j^{(k)}$ are the k-th component of sample points $\mathbf{x}_i$ and $\mathbf{x}_j$, respectively. $\mathbf{r}$ is the correlation vector of length m between the given input $\mathbf{x}$ and the samples $\{\mathbf{x}_1, \ldots, \mathbf{x}_m\}$, i.e., $\mathbf{r} = [R(\mathbf{x}, \mathbf{x}_1), R(\mathbf{x}, \mathbf{x}_2), \ldots, R(\mathbf{x}, \mathbf{x}_m)]^T$.

The estimation of the unknown parameters β and $\{\theta_k\}_{k=1}^n$ can be carried out using the maximum likelihood method [Shi and Rasheed, 2010]. Aside from the approximation values, Kriging model or Gaussian process can also provide a confidence interval without much additional computational cost incurred. However, one main disadvantage of Gaussian process is the significant increasing of computational expense when the dimensionality becomes high, due to the matrix inversions in the estimation of parameters.

Appendix B: Complexity Analysis and Parameters of EvoLS Framework

Here we comment on the computational complexity of present conventional surrogate selection schemes that take roots in the fields of statistical and machine learning [Fielding and Bell, 1997, Queipo et al., 2005, Tenne and Armfield, 2008a]. In conventional surrogate selection schemes, multiple sets of sample data are generally segregated, typically into training and test sets. For each approximation methodology, the respective surrogate model is commonly constructed based on the training set and the true error is estimated using the test set in the prediction process. This procedure of computation cost C_M is typically repeated for k times on different training and test sets to arrive at a statistically sound estimation of the approximation error that is then used in the selection scheme. Although many error estimation approaches are in abundance, the major differences lie mainly on how the training and test sets are generated, which vary from random subsampling (holdout), k-fold cross-validation and bootstrapping as described in [Kohavi, 1995]. For ID number of approximation methodologies considered, the overall computational complexity of the conventional selection scheme in estimating the error of the surrogates can thus be derived as $O(ID \times k \times C_M)$.

Next, a complexity analysis of the EvoLS framework is detailed. Apart from the standard parameters of a typical surrogate-assisted evolutionary algorithm [Lim et al., 2010], EvoLS has two additional parameters: database $\Phi_{M_{id}}$ and density function $P(\mathbf{y}|\mathbf{P}^t, \mathbf{x})$. Typically, the form of $P(\mathbf{y}|\mathbf{P}^t, \mathbf{x})$ can be explicitly defined according to the stochastic operator used (as illustrated in Section 3), while databases $\Phi_{M_{id}}$ naturally follows a first-in-first-out queue structure to favor more recently archived optimization data $\{(\mathbf{y}, \varphi_{M_{id}}(\mathbf{y}))\}$. The complexity for *evolvability* learning of surrogates can be derived as $O(ID \times |\Phi_{M_{id}}| \times C_E)$ where $|\Phi_{M_{id}}|$ denotes the database size, ID denotes the number of approximation methodologies used, and C_E is the computational effort incurred to determine $P(\mathbf{y}_i|\mathbf{P}^t, \mathbf{x})$ for each $\mathbf{y}_i$. For each individual, since only the most productive approximation methodology inferred is used to construct a new surrogate at a computational requirement of C_M, the complexity of EvoLS can be derived as

$O(ID \times |\Phi_{M_{id}}| \times C_E + C_M)$. Nevertheless, as $(ID \times |\Phi_{M_{id}}| \times C_E) << C_M$ in practice, the computational complexity of EvoLS becomes $O(C_M)$. Thus, EvoLS offers an alternative to the conventional selection scheme with a significantly lower complexity of $O(C_M)$ that is independent of the number of approximation methodologies considered in the framework.

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