Fitness Approximation in Evolutionary Computation - A Survey

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Abstract

Fitness evaluation is a basic operation in evolutionary computation. However, an explicit fitness function is not always available in real-world applications. In many cases, it is necessary to estimate the fitness function by constructing an approximate model. In this paper, a short survey on fitness approximation in evolutionary computation is given. Main issues like approximation models, model management schemes, learning methods as well as data sampling techniques are presented. Finally, interesting open problems are discussed.

1 Introduction

Evolutionary algorithms are receiving increasing interest both in academy and industry. Among other applications, evolutionary algorithms have been widely used as global optimizers. Generally, evolutionary algorithms outperform conventional optimization algorithms for problems which are discontinuous, non-differential, multi-modal, noisy and not well-defined problems, such as art design, music composition and experimental designs [47]. Besides, evolutionary algorithms are also well suitable for multi-criteria problems.

With all the great successes achieved in real-world applications, evolutionary algorithms have also encountered some challenging difficulties. For most evolutionary algorithms, a large number of fitness evaluations (performance calculations) are needed before a well acceptable solution can be found. In many real-world applications, fitness evaluation is not trivial. There are several situations in which fitness evaluation becomes difficult and a computationally efficient approximate model (also known as meta-model) will be very helpful.

If an approximate model is needed for fitness evaluation, an important issue is then to select the most important one for fitness approximation. So far, there are several models that can be used for fitness approximation. The most popular ones are polynomials (often known as Response Surface Methodology), the kriging model, also known as design and analysis of computer experiments (DACE) and feedforward neural networks, including multi-layer perceptrons and radial-basis-function networks. Due to the lack of data and the high dimensionality of input space, it is very difficult to obtain a perfect global approximation of the original fitness function. To address this problem, two main measures can be taken. Firstly, the approximate model should be used together with the original fitness function. In most cases, the original fitness function is available, although it is computationally very expensive. Therefore, it is very important to use the original fitness function efficiently. This is called evolution control [24] or model management. Secondly, the quality of the approximate model should be improved as much as possible given a limited number of data. Several aspects are important to improve the model quality, such as selection of the model, use of active data sampling and weighting (both on-line and off-line), selection of training method and selection of error measures.

The work on fitness approximation in evolutionary computation has been distributed in several different areas. Therefore, this survey aims at providing readers a relatively comprehensive picture of fitness approximation in evolutionary computation. In Section 2, different motivations for using approximation in evolutionary computation are presented. The issue of model management is described in Section 3, where existing methods are divided into three main schemes. The main approximation models that have been used in fitness approximation are introduced in Section 4. Data

sampling techniques, which are very important for the quality of models, are given in Section 5. Finally, open questions and promising research topics are discussed in Section 6.

2 Motivations

The concept of approximation in optimization is not new [1]. Generally, there are two basic approaches, i.e., functional approximation and problem approximation. In functional approximation, an alternate and explicit expression is constructed for the objective function (in evolutionary computation, it is usually called fitness function). In contrast, problem approximation tries to replace the original statement of the problem by one which is approximately the same to the original problem but which is easier to solve. In this survey, the main focus is function approximation, nevertheless, the issue of problem approximation will also be discussed briefly in the last section.

So far, approximation of the fitness function in evolutionary computation has been applied mainly in the following cases.

- The computation of the fitness is extremely time-consuming. One good example is structural design optimization [19, 30, 29, 21, 34, 48, 38, 25]. In aerodynamic design optimization, it is often necessary to carry out computational fluid dynamics (CFD) simulations to evaluate the performance of a given structure. A CFD simulation is usually computationally expensive, especially if the simulation is 3-dimensional, which takes over ten hours on a high-performance computer for one calculation. Therefore, approximate models have widely been used in structure optimization [1].

  Fitness approximation has also been reported in protein structure prediction using evolutionary algorithms [35, 37]. A neural network has been used for feature extraction from amino acid sequence in evolutionary protein design [46].

- There is no explicit model for fitness computation. In many situations, such as in art design and music composition as well as in some areas of industrial design, the evaluation of the fitness depends on the human user. Generally, these problems can be addressed using interactive evolutionary computation [50]. However, a human user can easily get tired and an approximate model that embodies the opinions of the human evaluator is also very helpful [2, 27].

- The environment of the evolutionary algorithm is noisy. Usually, there are two methods to deal with noisy fitness functions. The first one is to sample the fitness several times and to average [16]. However, this method requires a large number of additional fitness evaluations. The second method is to calculate the fitness of an individual by averaging the value of this individual as well as that of other individuals in its neighborhood. To avoid additional computational cost, the individuals that participate in the averaging can be chosen from the current and previous generations [5]. A more flexible alternative is to estimate the fitness of the individuals in the neighborhood using a statistical model constructed with history data [45, 6].

- The fitness landscape is multi-modal. The basic assumption is that a global model can be constructed to approximate and smoothen out the local optima of the original multi-modal fitness function without changing the global optimum and its location [31]. Similar ideas have also been reported in conventional optimization methods [3, 4]. However, it is generally difficult to build an approximate model that has the same global optimum on the same location when the dimensionality is high with limited number of samples.

3 Approximate Model Management

The application of approximation models to evolutionary computation is not as straightforward as one may expect. There are two major concerns in using approximate models for fitness evaluation. First, it should be ensured that the evolutionary algorithm converges to the global optimum or a near-optimum of the original fitness function. Second, the computational cost should be reduced as much as possible. One essential point is that it is very difficult to construct an approximate model that is globally correct due to the high dimensionality, ill distribution and limited number of training samples. It is found that if an approximate model is used for fitness evaluation, it is very likely that the evolutionary algorithm will converge to a false optimum. A false optimum is an optimum of the approximate model, which is not one of the original fitness function, refer to Fig.1 for an example. Therefore, it is very essential in most cases that the approximate model should be used together with the original fitness function. This can be regarded as the issue of model management or evolution control. By evolution control, it is meant that in evolutionary computation using approximate models, the original fitness function is used to evaluate some of the individuals or all indi-

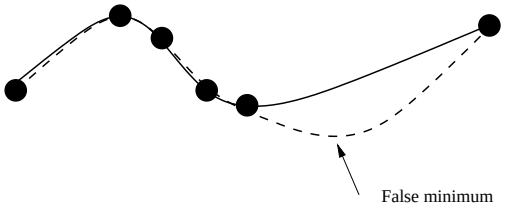

Figure 1: An example of a false minimum in the approximate model. Solid line denotes the original fitness function, dashes line the approximate model and the dots the available samples.

viduals in some generations [24]. An individual that is evaluated using the original fitness function is called a controlled individual. Similarly, a generation in which all its individual are evaluated using the original fitness function is called a controlled generation.

Generally, existing work on approximation in evolutionary computation can be divided into three main approaches from the viewpoint of evolution control.

3.1 No Evolution Control

Very often, the approximate model is assumed to be of high-fidelity and therefore, the original fitness function is not at all used in evolutionary computation, such as in [2, 43, 27].

3.2 Fixed Evolution Control

The importance to use both the approximate model and the original function for fitness evaluation has been recognized [41]. There are generally two approaches to evolution control, one is individual-based [19, 10], and the other is generation-based [41, 42]. By individual-based control, it is meant that in each generation, some of the individuals use the approximate model for fitness evaluation and others the original function for fitness evaluation. In individual-based evolution control, either a random strategy or a best strategy can be used to select the individuals to be controlled [24]. In the best strategy, the best individual (based on the ranking evaluated by the approximate model) in the current generation is reevaluated using the original function [19], see Fig.2. To reduce the computational cost further, individual-based evolution control can be carried out only in a selected number of generations [10]. In contrast, the random strategy selects certain number of individuals randomly for reevaluation using the original fitness function [24]. An alternative to the best strategy and the random strategy is to evaluate the mean of the individuals in the current population [34].

Generation-based evolution control can also be implemented [41, 42]. In [41], generation-based evolution control is carried out when the evolutionary algorithm converges on the approximate model. More heuristically, evolution control is carried out once in a fixed number of generations, see Fig. 3.

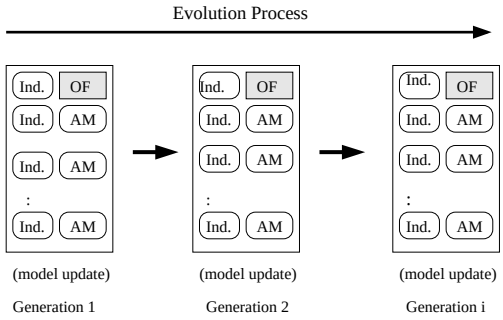

Figure 2: The best individual is controlled in each generation. AM: approximate model; OF: original function.

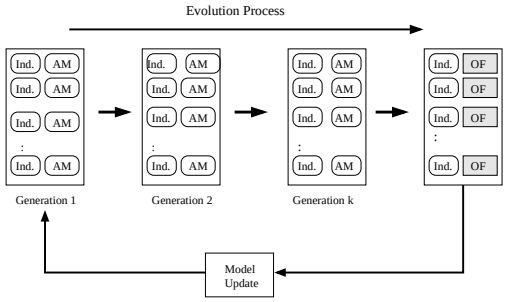

Figure 3: Generation-based evolution control. AM: approximate model; OF: original function.

One drawback in the aforementioned methods is that the frequency of evolution control is fixed. This is not very practical because the fidelity of the approximate model may vary significantly during optimization. In fact, a predefined evolution control frequency may cause strong oscillation during optimization due to large model errors, as observed in [41].

3.3 Adaptive Evolution Control

It is straightforward to imagine that the frequency of evolution control should depend on the fidelity of the approximate model. A method to adjust the frequency of evolution control based on the trust region framework [14] has been suggested in [34], in which the generation-based approach is used. A framework for approximate model management has also been suggested in [25], which has successfully been applied to 2-dimensional aerodynamic design optimization, see Fig. 4.

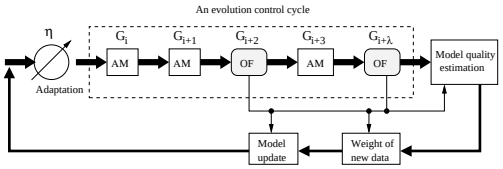

Figure 4: Adaptive generation-based evolution control. In the evolution control cycle, there are λ generations, η ($\eta \leq \lambda$) generations will be controlled. AM: approximate model; OF: original function.

4 Approximation Models

4.1 Polynomial Models

The most widely used polynomial approximation model is the second-order model which has the following form:

$$\hat{y} = \beta_0 + \sum_{1 \leq i \leq n} \beta_i x_i + \sum_{1 \leq i \leq j \leq n} \beta_{n-1+i+j} x_i x_j, \quad (1)$$

where β_0 and β_i are the coefficients to be estimated, and the number of terms in the quadratic model is $n_t = (n+1)(n+2)/2$ in total, where n is the number of input variables.

To estimate the unknown coefficients of the polynomial model, both least square method (LSM) and gradient method can be used:

- **Least Square Method** To get a unique estimation of the coefficients using LSM, it is required that the number of samples (N) drawn from the original function should be equal to or larger than the number of coefficients n_t. Let

$$\boldsymbol{y} = [y^{(1)}, y^{(2)}, \cdots, y^{(N)}]^T, \quad (2)$$

and

$$\boldsymbol{X} = \begin{bmatrix} 1 & x_1^{(1)} & x_2^{(1)} & \cdots & (x_n^{(1)})^2 \\ 1 & x_1^{(2)} & x_2^{(2)} & \cdots & (x_n^{(2)})^2 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{(N)} & x_2^{(N)} & \cdots & (x_n^{(N)})^2 \end{bmatrix}, \quad (3)$$

then the following equation holds:

$$\boldsymbol{y} = \boldsymbol{X}\boldsymbol{\Theta}, \quad (4)$$

The LSM algorithm works as follows,

$$\hat{\boldsymbol{\Theta}} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y}, \quad (5)$$

where $\hat{\boldsymbol{\Theta}}$ denotes the estimate of $\boldsymbol{\Theta}$. One assumption here is that the rows of $\boldsymbol{X}$ are linearly independent.

- **Gradient Method** The main drawback of the least square method is that the computational expense becomes unacceptable as the dimensionality increases. To address this problem, the gradient method can be used. Define the following square error function for the k-th sample:

$$E^{(k)} = \frac{1}{2}(y - y^{(k)})^2, \quad (6)$$

where y is defined in equation (1), it is then straightforward to get the update rule for the unknown coefficients:

$$\begin{aligned} \Delta\beta_0 &= -\xi \cdot (y - y^{(k)}) & (7) \\ \Delta\beta_i &= -\xi \cdot (y - y^{(k)}) x_i^{(k)} & (8) \\ \Delta\beta_{n-1+i+j} &= -\xi \cdot (y - y^{(k)}) x_i^{(k)} x_j^{(k)}, & (9) \\ & \quad 1 \leq i \leq j \leq n. \end{aligned}$$

4.2 Kriging Models

The kriging model can be seen as a combination of a global model plus a localized "deviation":

$$y(\boldsymbol{x}) = g(\boldsymbol{x}) + Z(\boldsymbol{x}), \quad (10)$$

where $g(\boldsymbol{x})$ is a known function of $\boldsymbol{x}$ as a global model of the original function, and $Z(\boldsymbol{x})$ is a Gaussian random function with zero mean and non-zero covariance that represents a localized deviation from the global model. Usually, $g(\boldsymbol{x})$ is a polynomial and in many cases, it is reduced to a constant β.

The covariance of $Z(\boldsymbol{x})$ is expressed as

$$\begin{aligned} \mathrm{Cov}[Z(\boldsymbol{x}^{(j)}), Z(\boldsymbol{x}^{(k)})] &= \sigma^2 \boldsymbol{R}[R(\boldsymbol{x}^{(j)}, \boldsymbol{x}^{(k)})] & (11) \\ & \quad j, k = 1, \cdots, N, \end{aligned}$$

where R is the correlation function between any two of the N samples, and $\boldsymbol{R}$ is the symmetric correlation matrix of dimension $N \times N$ with values of unity along the diagonal. The form of the correlation matrix can be selected by the user, and the following form has often been used [9, 18, 49]:

$$R(\boldsymbol{x}^{(j)}, \boldsymbol{x}^{(k)}) = \exp[-\sum_{i=1}^{n} \theta_i |x_i^{(j)} - x_i^{(k)}|^2], \quad (12)$$

where θ_i are the unknown correlation parameters, $x_i^{(j)}$ and $x_i^{(k)}$ are the i-th component of sample points $\boldsymbol{x}^{(j)}$ and $\boldsymbol{x}^{(k)}$. Thus, the prediction of $y(\boldsymbol{x})$ is a function of unknown parameters β and $\theta_i, i = 1, 2, \cdots, n$:

$$\hat{y} = \hat{\beta} + \boldsymbol{r}^T(\boldsymbol{x})\boldsymbol{R}^{-1}(\boldsymbol{y} - \beta\boldsymbol{I}), \quad (13)$$

where, $\hat{y}$ is the estimated value of y given the N samples and the current input $\boldsymbol{x}$, $\hat{\beta}$ is the estimated value of β, $\boldsymbol{y}$ is a vector of length N as defined in Eqn. (2), $\boldsymbol{I}$ is a unit vector of length N, and $\boldsymbol{r}$ is the correlation vector of length N between the given input $\boldsymbol{x}$ and the samples $\{\boldsymbol{x}^{(1)}, \cdots, \boldsymbol{x}^{(N)}\}$:

$$\boldsymbol{r}^T(\boldsymbol{x}) = [R(\boldsymbol{x}, \boldsymbol{x}^{(1)}), R(\boldsymbol{x}, \boldsymbol{x}^{(2)}), \cdots, R(\boldsymbol{x}, \boldsymbol{x}^{(N)})]^T. \tag{14}$$

The estimation of the parameters can be carried out using the maximum likelihood method. Note that it is necessary to perform matrix inversions for estimating the output in the kriging model, which increases the computational expense significantly when the dimensionality becomes high.

4.3 Neural Networks

Neural networks have shown to be effective tools for function approximation. Both feedforward multilayer perceptrons and radial-basis-function networks have widely been used.

- **Multilayer perceptrons** An MLP with one input layer, two hidden layers and one output neuron can be described by the following equation:

$$y = \sum_{l=1}^{L} v_l f(\sum_{k=1}^{K} w_{kl}^{(2)} f(\sum_{i=1}^{n} w_{ik}^{(1)} x_i)), \tag{15}$$

  where, n is the input number, K and L are the number of hidden nodes, and $f(\cdot)$ is called activation function, which usually is the logistic function

$$f(z) = \frac{1}{1 + \mathrm{e}^{-az}}, \tag{16}$$

  where a is a constant.

- **Radial-Basis-Function Networks** The theory of radial-basis-function (RBF) networks can also be tracked back to interpolation problems [40]. An RBF network with one single output can be expressed as follows:

$$y(\boldsymbol{x}) = \sum_{j=1}^{N} w_j \boldsymbol{\phi}(\| \boldsymbol{x} - \boldsymbol{x}^{(j)} \|), \tag{17}$$

  where $\boldsymbol{\phi}(\cdot)$ is a set of radial-basis functions, $\| \cdot \|$ is usually a Euclidean norm, the given samples $\boldsymbol{x}^{(j)}, j = 1, \cdots, N$ are the centers of the radial-basis function, and w_j are unknown coefficients. However, this model is expensive to implement if the number of samples is large. Therefore, a generalized RBF network is more practical

$$y(\boldsymbol{x}) = \sum_{j=1}^{L} w_j \boldsymbol{\phi}(\| \boldsymbol{x} - \boldsymbol{\mu}^{(j)} \|). \tag{18}$$

  The main difference is that the number of hidden nodes (L) is ordinarily smaller than the number of samples (N), and the centers of the basis functions ($\boldsymbol{\mu}^{(j)}$) are also unknown parameters that have to be learned. Usually, the output of a generalized RBF network can also be normalized:

$$y(\boldsymbol{x}) = \frac{\sum_{j=1}^{L} w_j \boldsymbol{\phi}(\| \boldsymbol{x} - \boldsymbol{\mu}^{(j)} \|)}{\sum_{j=1}^{L} \boldsymbol{\phi}(\| \boldsymbol{x} - \boldsymbol{\mu}^{(j)} \|)}. \tag{19}$$

4.4 Comparative Remarks

There are several papers that compare the performance of different approximation models [11, 12, 18, 49, 48, 23]. However, no clear conclusions on the advantages and disadvantages of the different approximation models have been drawn. This is reasonable not only because the performance may depend on the problem to be addressed, but also because more than one criterion needs to be considered. The most important factors are accuracy, both on training data and test data, computational complexity and transparency. It has been found in [24] that an approximate model may introduce false optima, although it has very good performance on the training data, refer to Fig. 1. This is more harmful than a lower approximation accuracy if the model is used in global optimization such as evolutionary optimization. Methods to prevent a neural network model from generating false minima have been suggested in [24], which are very effective for lower dimensional problems.

Although it is difficult to provide explicit rules on model selection, some general remarks can still be made on different approximation models. Firstly, it is recommended to implement first a simple approximate model for a given problem, for example, a lower order polynomial model to see if the given samples can be fit reasonably. If a simple model is found to underfit the samples, a model with higher complexity should be considered, such as higher order polynomials or neural network models. However, if the input space (design space) is high-dimensional and the number of samples is limited, a neural network model is preferred. It is recalled that to estimate the unknown parameters of a second-order polynomial model, at least $(n + 1) \times (n + 2)/2$ data samples are required. Otherwise, the model will be undetermined.

Secondly, if a neural network model, in particular a multilayer perceptrons network is used, it is necessary

to consider regulating the model complexity to avoid overfitting. It may also be necessary to try other more efficient training methods [44] if the gradient descent based method is found to be of slow convergence. Besides, RBF networks have found to be of good accuracy as well as of fast training in some studies [48, 23].

5 Data Sampling Techniques

If an approximate model is used for evolutionary computation, both off-line and on-line training will be involved if the evolution is controlled. Off-line learning denotes the training process before the model is used in evolutionary computation. In contract, on-line learning denotes the update of the model during optimization. Usually, the samples for off-line learning can be generated using Monte-Carlo method, however, it has been shown in different research areas that active selection of the samples will improve the model quality significantly. During on-line learning, data selection is strongly related to the search process.

5.1 Off-line Data Sampling

Several data sampling methods have been suggested in the fields of design of experiments [33, 20], statistics and machine learning. Some popular methods are:

- **Design of experiments (DOE)** Orthogonal arrays (OA), central composite designs (CCD), and D-optimality are most widely used in design of experiments. A first-order orthogonal design is one for which $\boldsymbol{X}^T\boldsymbol{X}$ is a diagonal matrix, where $\boldsymbol{X}$ is the extended sample array as defined in Eqn. (3). In other words, the columns of $\boldsymbol{X}$ are mutually orthogonal.

  Central composite design enables the efficient construction of second-order polynomial models. CCDs are basically first-order (2^n) designs augmented by $2n$ additional center and "star" points to allow estimation of the coefficients of a second-order model. An example of CCD designs is given in Fig. 5 for a two-dimensional problem.

  D-optimality takes advantage of the properties of polynomial models in data sampling. The accuracy of the least square estimate in Eqn. (5) is defined as:

$$\mathrm{Var}(\hat{\Theta}) = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\sigma^2, \qquad (20)$$

  where σ^2 is the variance of the estimate error. From Eqn. (20), it can be seen that to improve the quality of fit, one should maximize the determinant of $\boldsymbol{X}^T\boldsymbol{X}$. Therefore, the D-optimality is to select the samples in such a way that the determinant of $\boldsymbol{X}^T\boldsymbol{X}$ is maximized. Although developed from the polynomial models, the D-optimality has also shown to be beneficial in data selection for constructing neural networks [13].

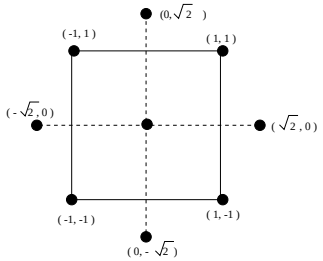

Figure 5: Central composite designs for $n = 2$. The dots represent the sample points. The samples on the solid lines are the first-order design and those on the dashed lines are central and star points ($\sqrt{n}$).

- **Active Learning** Active learning has widely been studied in the field of neural network learning [32, 51, 28]. The basic idea is to select the location of the next sampling data in such a way that an objective function is optimized. The objective function can be information gain, entropy reduction, or generalization error. It has been shown that active data selection can improve the generalization ability of neural networks without increasing the number of training samples.

5.2 On-line Data Sampling

Active data selection is also important in the case that the training data has been collected and therefore, the target is how to select a subset of the data for efficient training.

- **Bagging and boosting** Bagging [7] and boosting [17] are two statistical learning methods that have been developed to improve the quality of approximate model using bootstrap techniques [15]. In bagging (bootstrap aggregating), a number of bootstrap models are constructed using different bootstrap samples and the final output is the average of the models. It is shown that bagging is able to reduce the variance of estimate error efficiently. An adaptive bagging technique can reduce both variance and bias [8].

  Boosting algorithms are able to boost a weak learning algorithm into a strong one. A weak algorithm can be inaccurate rules of thumb that are slightly better than a random guess. The main

difference between boosting and bagging is that in boosting, the bootstrap samples are affected by the performance of the current model. In addition, the final output is a weighted average of the different models.

- **Active data selection** Some of the statistical active learning methods can also be applied to this type of data selection [39]. A special case of integrated mean square error, called integrated squared bias is used as the criterion to select a subset from available data to improve learning performance. However, it is assumed that the data is noiseless.

- **Data weighting guided by evolution** In [25], a method to weight the available data using the information from the evolutionary algorithm has been suggested. The basic idea is that if information on search direction of the evolutionary algorithm is available, then a larger weight should be given to the data samples located in the region where the evolutionary algorithm will most probably visit in the next generation.

  In [42], several strategies for data sampling have been studied. For example, some strategies use the best individuals to replace the worse ones in the training samples, or the ones that are randomly selected. Some strategies create new points randomly and replace the worst ones in the training samples. It has been found that the strategy that simply re-evaluates the best individuals (best in the sense of the approximate model) with the original fitness function exhibits the best performance. This is actually the best strategy in individual-based evolution control.

6 Discussions

Fitness approximation in evolutionary computation is a research area that has not yet attracted sufficient attention in the evolutionary computation community. In fact, the following points still need to be clarified:

- Although several studies have shown very promising results using approximate models in evolutionary computation, it is theoretically still unclear in which way the evolutionary algorithm can benefit from the approximate model. In the least sense, as pointed out in [42], the approximate model can prevent the information in the history of optimization from being lost, although approximate models themselves do not create new information.

- Which type of models helps most, a local one or a global one? It is straightforward to imagine that a global model is able to simplify the search process if the approximate model does not change the properties of the original fitness function. However, from the viewpoint of model construction, to build a local model is much more feasible than to build a global model.

In addition, there are also several topics that deserve further research. Some of them are:

- Development of learning algorithms that are efficient and less sensitive to the number of training data. Learning of problem class [22] and incorporation of *a priori* knowledge [26] are two possible approaches.

- Approximate model with a variable input dimension. During optimization, the input dimension may change in many cases. For example, if an adaptive representation is used in design optimization, the number of parameters increases or decreases during optimization [36].

- Management of different levels of approximation. So far, only functional approximation has been discussed. However, there are different levels of problem approximation in many applications. For example, in computational fluid dynamics simulation, 2D Euler-Lagrange equations, Navier-Stokes equations, quasi 3D simulations and 3D simulations are different approximations of the original problem. Thus, combining different levels of approximation with the approximate model is very interesting.

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