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Two-level Multi-surrogate Assisted Optimization method for high dimensional nonlinear problems

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ABSTRACT

Curse of dimensionality is a key issue in engineering optimization. When the dimension increases, distribution of samples becomes sparse due to expanded design space. To obtain accurate and reliable results, the amount of samples often grows exponentially with the dimensions. To improve the efficiency of the surrogate with limited samples, a Two-level Multi-surrogate Assisted Optimization (TMAO) is suggested. The framework of the TMAO is to decompose a complicated problem into separable and non-separable components. In the first-level, High Dimensional Model Representation (HDMR) is utilized to determine the correlations among input variables. Then, a high dimensional problem can be decomposed into separable and non-separable components. Thus, the dimension of the original problem might be reduced significantly. Moreover, considering noises and outliers, Support Vector Regression (SVR)-HDMR is utilized to obtain more reliable surrogate. Expected Improvement (EI) criterion is suggested to generate new samples to save computational cost. In the second-level, to handle the non-separable component, a multi-surrogate assisted sampling strategy is suggested. Compared with other methods, the distinctive characteristic of the suggested sampling strategy is to use different surrogates to search potential uncertain regions. Considering the diversity of surrogates, more feature samples might be generated close to the local optimum. Even though it is still difficult to find a global solution, it could help us to find a feasible solution in practice. To verify the performance of the suggested method, several high dimensional mathematical functions are tested by the suggested method. The results demonstrate that all test functions can be successfully solved.

1. Introduction

In the past 30 years, Surrogate Assisted Optimization (SAO) methods have been extensively used in multidiscipline. The SAO is invoked as a substitution for physical models or simulation-based evaluations, improving the efficiency of optimization procedure significantly. However, with the development of complexity of practical engineering design, it is difficult for the SAO to handle such complicated problems, especially for high dimensional problems. Generally, the essential of SAOs is approximation. To improve the performance of surrogate in terms of accuracy and reliability, various surrogate modeling methods have been developed and applied in various disciplines in the past 30 years, such as Polynomial Regression (PR) [1], Radial Basis Function (RBF) [2–4], Moving Least Square (MLS) [5,6], Kriging [7,8] and SVR [9,10]. The most influential SAO might be Efficient Global Optimization (EGO) developed by Jones et al. [11], which can be utilized to find global optimization assisted by Kriging. Chen et al. used heuristics method

Abbreviations: AI, Artificial Immune; EICAM, EI criterion assisted modeling; EGO, Efficient Global Optimization; EI, Expected Improvement; GA, Genetic Algorithm; GMDH, Group Method of Data Handling; GSS, Golden Section Sampling; HDMR, High Dimensional Model Representation; LOOCV, Leave-One-Out Cross Validation; MAS, Multi-surrogate Assisted Sampling algorithm; EImax, maximum EI; MLS, Moving Least Square; NTS, Number of Test Samples; PR, Polynomial Regression; PSO, Particle Swarm Optimization; RAAE, Relative Average Absolute Error; RBF, Radial Basis Function; RMAE, Relative Maximum Absolute Error; SA, Simulated Annealing; STD, Standard Deviation; SAEO, Surrogate Assisted Evolutionary Optimization; SAO, Surrogate Assisted Optimization; SVR, Support Vector Regression; TMAO, Two-level Multi-surrogate Assisted Optimization; TLBO, Teaching Learning-Based Optimization.

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to lead the surface refinement to a smaller design space [12]. Wujek and Renaud compared a number of move-limit strategies which focused on controlling function approximation in a more "meaningful" design space [13,14]. Alexandrov et al. advocated the use of a sequential modeling approach using Trust Region Method (TRM) [15]. Rodríguez employed trust region augment Lagrangian method for Sequential Response Surface Method (SRSM) [16]. Wang et al. developed an Adaptive RSM (ARSM), which systematically reduced the size of design space [17]. Wang et al. proposed a Boundary and Best Neighbor Sampling (BBNS)-based ARSM, which is integrated with the MLS approximation for nonlinear problems [18]. Another sub-branch of SAOs is Surrogate Assisted Evolutionary Optimization (SAEO). Studies on SAEOs began over two decades ago and have received considerably increasing interest in recent years. For the SAEOs, surrogates are commonly integrated with Evolutionary Algorithms (EAs), such as Genetic Algorithm (GA), Particle Swarm Optimization (PSO) and Teaching Learning-Based Optimization (TLBO) [19–21]. Theoretically, the surrogate can be applied to almost all operations of the EA, such as population initialization, cross-over, mutation and local search and fitness evaluations [22]. The SAEO commonly uses surrogates in the local search for both single and multi-objective optimization methods [23,24]. In such cases, sophisticated model management methods developed in traditional design optimization, such as TRM can be employed directly [25]. The surrogate has also been used in stochastic search methods other than EAs, such as surrogate assisted Simulated Annealing (SA) [26] or Artificial Immune (AI) systems [27]. Although SAOs have achieved good results for various disciplines, most of high dimensional nonlinear problems still cannot be handled, especially for costly simulation evaluations. According to Wang and Shan [28] and Chen et al.s' [29] suggestions, 10 or more dimensional problems can be considered high if the corresponding evaluation is time consuming, and such problems widely exist in various disciplines.

For a practical industrial design application, if all input variables are independent, each parameter can be designed individually. Ideally, under such circumstance, a complicated case can be decomposed easily. Practically, for most of the problems, design parameters are commonly correlated. However, according to application experiences, some of them are weak correlated. If the correlations among input variables can be identified, a high dimensional problem might be decomposed into a combination of some low or medium problems and can be solved easier than the original one. The HDMR is a particular family of representations where each term reflects the independent and cooperative contributions of inputs upon the output. The HDMR was elaborated by Rabitz et al. [30]. Similar to Taylor expansion, a HDMR expansion expresses a high dimensional function as a finite hierarchical correlated function expansion in terms of inputs, which can efficiently reduce sampling effort for learning the behavior of a high dimensional system and automatically identify the correlated relationship among input variables. Recently, Shorter et al. utilized the HDMR to build an efficient chemical kinetics solver [31]. Li et al. proposed a HDMR-based random sampling method and developed an approach to approximate its different component functions [32]. Shan and Wang integrated RBF with cut-HDMR for high dimensional expensive black-box problems [33]. Wang et al. utilized the MLS as a basis function for cut-HDMR and applied to high dimensional problems [34]. However, the HDMR is still rather a modeling technique than an optimizer. If a practical case is optimized by HDMRs, the computational cost is still expensive.

To improve the performance of HDMRs and make them feasible for optimizer, a Two-level Multi-surrogate Assisted Optimization (TMAO) method is suggested. Compared with other HDMRs, the HDMR is only a decomposer for the original problem in the TMAO. Even for a non-separable problem, it still can be solved by other strategies in such framework. Generally, in the first-level, the HDMR is utilized to decompose the original input variables by considering noises and outliers. In this level, low correlated term (two-order) is considered. In the second-level, an ensemble sampling strategy is suggested for uncoupled variables based sub-problems. Therefore, the sub-solution can be obtained based on each decomposed sub-problem. To verify the feasibility and performance of the TMAO, several test functions are employed.

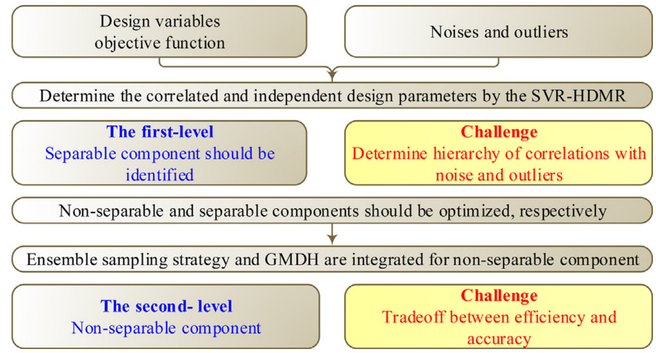

Fig. 1. The framework of TMAO and corresponding challenges.

2. Brief view of framework of TMAO and challenges

Mathematically, a high dimensional problem can be decomposed into two components, separable and non-separable components. For a separable component f_{sp}, it can be expressed as

$$\left\{ arg\left(\min_{x_1} f(x_1, \ldots)\right), \ldots, arg\left(\min_{x_n} f(\ldots, x_n)\right) \right\} = arg\left(\min_{x_1,\ldots,x_n} f(x_1 \ldots, x_n)\right). \tag{1}$$

It means that f_{sp} can be decomposed into n functions independently, and each function can be modeled or optimized individually. In other words, input variables of f_{sp} function are independent and can be expressed as

$$f_{sp}(x_1, \ldots, x_n) = \sum_{i=1}^{n} f_i(x_i). \tag{2}$$

If Eq. (2) is satisfied, it suggests that all input variables are independent and can be designed independently. Generally, the HDMR can help the designer to decompose a high dimensional function into several combinations of low or medium dimensional functions. Thus, the physical essential of an underlying system can be disclosed partly. Such a decomposed problem is easy to be solved compared with the original one. Therefore, the purpose of the first-level is reduction of dimensionality as shown in Fig. 1.

As shown in Fig. 1, the cut-HDMR is utilized to determine the correlations of input variables $x_i x_j$. Theoretically, all hierarchy of correlations can be identified by the cut-HDMR, such as $x_i x_j x_k$, $x_i x_j x_k \ldots x_z$. Obviously, the number of samples should be dramatically increased correspondingly. Fortunately, most of the practical problems are commonly low-order or weak high-order correlated, only $x_i x_j$ correlated terms are considered in most of HDMRs. The assumption is also used in the first-level of the TMAO. Compared with other HDMR-based optimization method, the errors due to loss of high-order correlated term can be compensated in the second level and should be discussed later.