A Surrogate-ensemble Assisted Coevolutionary Algorithm for Expensive Constrained Multi-Objective Optimization Problems

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***Abstract*—In real-world applications, there are some constrained multi-objective problems where the evaluation of objectives is expensive and the evaluation of constraints is cheap. Currently, few studies have focused on solving expensive constrained multi-objective optimization problems (ECMOPs), and they usually assume that the constraints of ECMOPs are also expensive. In this paper, we propose a surrogate-ensemble assisted coevolutionary algorithm (SEACoEA) for ECMOPs with inexpensive constraint evaluation. First, a feasible sampling strategy is designed to initialize the population in the feasible regions. Next, two populations are set to optimize the original ECMOP and the problem without considering constraints, respectively. To improve the search efficiency, we redesigned the objective function of the surrogate-ensemble model. Finally, a new infill strategy is proposed to select candidate individuals from each population for real evaluation. Experimental results show that the proposed algorithm performs significantly better on most MW problems compared to several state-of-the-art algorithms.**

***Index Terms*—Expensive Constrained multi-objective optimization, Inexpensive constraints, Coevolution, Surrogate Ensemble**

I. INTRODUCTION

In practical applications, many multi-objective optimization problems require expensive physical experiments or time-consuming simulation to evaluate candidate solutions, such as computational fluid dynamics (CFD) simulations [1] and structural optimization [2], which are called expensive multi-objective optimization problems (EMOPs). Surrogate assisted evolutionary algorithms (SAEA) provides an effective method to solve EMOPs. In general, the procedure of SAEA is to build a surrogate model based on the data obtained from expensive evaluations, then use multi-objective evolutionary algorithms to optimize the EMOPs by using the surrogate model, thus reducing the computational cost. Although SAEA has made great progress on expensive multi-objective optimization problems, most studies [3]–[9] only consider unconstrained EMOPs, and only a few studies [10]–[14] consider constrained ECMOPs, and these algorithms assume that each objective function and constrained function are expensive. However, there are some constrained multi-objective optimization problems where the evaluation of objectives is expensive and the evaluation of constraints is cheap. For example, in the neural architecture search task, due to the large amount of time required to train the neural network, it is very expensive to evaluate the accuracy, generalization, and other metrics that need to be tested on the validation set, but not expensive to compute its constraints, such as whether the model satisfies constraints like model size or model structure. It does not need to go through a network training stage, but can be evaluated after the model is built [15]. This class of problems also needs to be studied because if the optimization algorithm of EMOPs is used directly without considering the constraints, no matter how good the solutions obtained by the search is, it cannot be applied in practice if the constraints are not satisfied. If the inexpensive constraints are assumed to be expensive, the complexity of the optimization problem will be increased and the search efficiency of the algorithm will be reduced.

In recent years, ECMOPs have attracted the attention of some researchers and achieved some research results [16], [17]. For example, Deb et al. [10] proposed six algorithm frameworks, namely M1-M6, which include methods such as constructing a surrogate model for each objective and constraint function, aggregating multiple objective functions or constraint functions into one objective function and constructing a surrogate model for it. Wang et al. [18] used random forest as a surrogate model and combined with NSGA-II [19] to solve expensive constrained multi-objective combinatorial optimization problems. R. de Winter et al. [13] proposed SAMO-COBRA using RBF as a surrogate model and using hypervolume contribution as an optimization indicator. Blank et al. [20] proposed IC-SA-NSGA-II. IC-SA-NSGA-II uses Riesz s-Energy Sampling [21] to initialize the population in the feasible region. Then RBF is used as a surrogate model and NSGA-II as an optimizer to search for new promising solutions.

Since the ECMOPs studied in this paper is characterized by expensive objectives and inexpensive constraints, it can be studied by combining the techniques of constrained multi-objective evolutionary algorithm and the expensive multi-objective evolutionary algorithm. As mentioned above, the main technique to deal with the expensive multi-objective problem is the surrogate model. The surrogate-ensemble model has better accuracy and robustness [7], [22] compared to a single surrogate model. There are many researches on constrained multi-objective problems [23]–[27], among which coevolutionary algorithms are very popular in recent years. Coevolutionary algorithms can search the Pareto front of a problem more efficiently by setting multiple coevolutionary populations.

For example, Tian et al. [28] proposed CCMO, which helps the population to jump out of the local optimum and helps the population to get across the infeasible region by setting an auxiliary population to search the unconstrained Pareto front. Liu et al. proposed BiCo [29], which searches from the infeasible region to the constrained Pareto front (CPF) and from the feasible region to the CPF by an archive population and a main population, respectively, so that the algorithm can search the CPF faster by the information exchange between the two populations. Based on this, this paper proposes a surrogate-ensemble assisted coevolutionary algorithm, namely SEACoEA. First, the proposed feasible sampling strategy is used to initialize the populations in the feasible region and keep them well-diversified in the decision space. Next, a surrogate-ensemble model is built for each objective, the CCMO is used as an optimizer to search, and a new fitness evaluation function is designed to improve the search efficiency of the population. Finally, candidate solutions are selected for real evaluation, and these candidates are integrated into the archive set and the surrogate-ensemble model is updated. The main contributions of this paper are summarized as follows:

1) A surrogate-ensemble assisted coevolutionary algorithm is proposed which can converge to Pareto fronts in small feasible regions under a limited computational budget.
2) A feasible sampling strategy is proposed to initialize the population in the feasible region and maintain a good distribution in the decision space.
3) A new proxy function is designed for each objective to balance the efficiency of exploitation and exploration in the evolutionary process by combining RBF and Kriging model

The remainder of this paper is organized as follows. In Section II, the surrogate model and CCMO algorithm are introduced briefly. Section III describes the proposed SEACoEA algorithm in detail. Section IV shows the experimental results of the SEACoEA algorithm and several state-of-the-art algorithms on MW1-14 problems. Finally, conclusions are drawn in Section V.

II. PRELIMINARIES

A. Radial Basis Function

Radial basis function (RBF) is an interpolation method that has been widely used in science and engineering [30]. RBF predicts the output y of the input $\mathbf{x}$ by a weighted sum of basis functions. Given a data set $\{(\mathbf{x}_i, y_i), \mathbf{x}_i \in R^D, y_i \in R, i \in \{1, ..., N\}\}$, the RBF prediction $\hat{f}(\mathbf{x})$ for the input $\mathbf{x}$ is as follows:

$$\hat{f}(\mathbf{x}) = \sum_{i=1}^{N} \omega_i \phi(\mathbf{x} - \mathbf{x}_i) \tag{1}$$

where $\omega = \{\omega_1, \omega_2, ..., \omega_N\}$ is the weight coefficient, $\phi(\cdot)$ represents the basis function. The weight vector ω is calculated by the following equation:

$$\omega = (\Phi^T \Phi)^{-1} \Phi^T \mathbf{y} \tag{2}$$

where $\mathbf{y} = (y_1, y_2, ..., y_N)^T$ is the output vector of the data-set, and Φ is defined as follows:

$$\Phi = \begin{bmatrix} \phi(\mathbf{x}_1 - \mathbf{x}_1) & \cdots & \phi(\mathbf{x}_1 - \mathbf{x}_N) \\ \vdots & \ddots & \vdots \\ \phi(\mathbf{x}_N - \mathbf{x}_1) & \cdots & \phi(\mathbf{x}_N - \mathbf{x}_N) \end{bmatrix} \tag{3}$$

B. Kriging Model

The Kriging model is also known as a Gaussian process. The Kriging model considers the inputs x and outputs y as random variables subject to a Gaussian distribution $\mathcal{N}(\mu, \sigma)$, where μ is the mean of the prediction, and σ is the variance of prediction, also known as uncertainty. Given a data set $\{(\mathbf{x}_i, y_i), \mathbf{x}_i \in R^D, y_i \in R, i \in \{1, ..., N\}\}$, the predicted value of the Kriging model for the input $\mathbf{x}$ can be expressed as follows:

$$\begin{aligned} \hat{f}(\mathbf{x}) &= \hat{\mu} + \mathbf{r}^T \mathbf{C}^{-1} \mathbf{y} - \mathbf{1}\hat{\mu} \\ \hat{\sigma}(\mathbf{x}) &= \hat{\sigma}^2 \left(1 - \mathbf{r}^T \mathbf{C}^{-1} \mathbf{r} + \frac{1 - (\mathbf{r}^T \mathbf{C}^{-1} \mathbf{r})^2}{\mathbf{1}^T \mathbf{C}^{-1} \mathbf{1}} \right) \end{aligned} \tag{4}$$

where $\mathbf{C}$ represents the covariance matrix of the data set, and $\mathbf{r}$ is the covariance vector of input $\mathbf{x}$ and training data $\mathbf{X}$. $\hat{\mu}$ and $\hat{\sigma}$ are calculated as follows:

$$\begin{aligned}\hat{\mu} &= \frac{\mathbf{1}^T\mathbf{C}^{-1}\mathbf{y}}{\mathbf{1}^T\mathbf{C}^{-1}\mathbf{1}} \\ \hat{\sigma} &= \frac{(\mathbf{y}-\mathbf{1}\hat{\mu})^T\mathbf{C}^{-1}(\mathbf{y}-\mathbf{1}\hat{\mu})}{N}\end{aligned} \tag{5}$$

C. CCMO

CCMO is a coevolutionary framework that sets up two populations, $Population1$ and $Population2$, to search for the original CMOP and helper problem, respectively. The two populations perform coevolution by combining their offspring populations to search the Pareto front of the original CMOP. The process of CCMO is shown in figure 1. Specifically, CCMO chooses a MOEA as the search algorithm, and in this paper NSGA-II is selected. First, it initializes $Population1$ and $Population2$, respectively. Then, the offsprings are generated by using the MOEA operators. During the evolutionary process, $Population1$ and $Population2$ are combined with the offspring of the two populations, respectively, and then $Population1$ and $Population2$ are updated using a MOEA's environmental selection mechanism. Finally, $Population1$ is output.

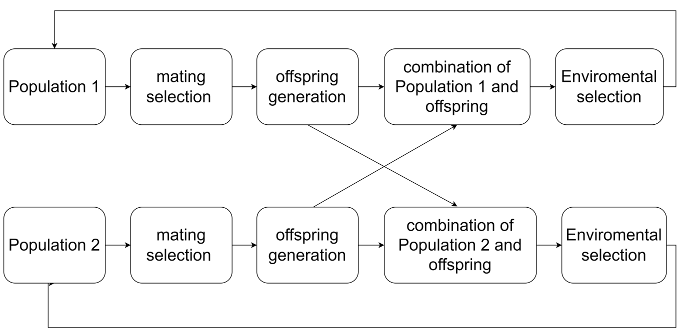

Fig. 1. The framework of CCMO [28]

III. The Proposed Algorithm

In this paper, we propose a surrogate-ensemble assisted coevolutionary algorithm called SEACoEA for CMOPs with inexpensive constraints and expensive objectives. First, a feasible sampling strategy is used to initialize the population so that the initial population are feasible solutions. The initialized population is assigned to $Population1$ and $Population2$. Next, a surrogate-ensemble model is built by using the real evaluated population. Then the surrogate-ensemble model and CCMO are used to guide the coevolution of $Population1$ and $Population2$. The candidate solutions are selected by the proposed selection strategy for real evaluation. Finally, the real evaluated individuals are added to the archive and the surrogate-ensemble model is updated by using these individuals. $Population1$ and $Population2$ are then updated by environmental selection mechanism, respectively. The feasible sampling strategy is described in Section III.A. The surrogate-ensemble assisted optimization is described in Section III.B. The infill strategy is described in Section III.C.

A. Feasible Sampling Strategy

Blank et al. first proposed IC-SA-NSGA-II [20] for CMOPs with inexpensive constraints and expensive objectives. IC-SA-NSGA-II uses three methods to initialize the population, including rejection based sampling, niching genetic algorithm and Riesz s-Energy optimization. However, the rejection sampling method is difficult to guarantee a better distribution of the population. The niching genetic algorithm needs to constantly adjust the niche size and run iteratively until enough feasible solutions are searched, which usually takes a long time to complete the sampling. The Riesz s-Energy optimization is difficult to extract enough feasible solutions in an acceptable time when the constraints are complex.

In view of this, this paper proposes a sampling strategy which can sample enough feasible solutions in a short time and maintain a good distribution of the initial population in the decision space. First, the constraint violation value is used as the optimization objective, and the genetic algorithm (GA) is used for optimization. An archive set is used to record the feasible individuals obtained during the search. Since the constraint violation value of the problem is used as the optimization objective, the sampling of the initial population becomes a single objective optimization problem. In order to maintain the distribution of the population in the decision space, a niche range $Size_{niche}$ is set for each individual in the archive set, and the offspring in this range will be eliminated to ensure the distribution of the sampled population in the decision space. When the number of feasible solutions in the population exceeds the population size, some individuals will be eliminated according to the descending order of generation that individuals enter the population, that is, the earlier feasible individual enter the population, the more probability it is to eliminate. Finally, a set of feasible individuals is selected from the archive set by K-means clustering algorithm. The pseudocode of the feasible sampling strategy is shown in Algorithm 1.

The population is initialized by Latin Hypercube sampling and the feasible solutions are merged into archive (lines 1 to 3). The offspring are generated using genetic operators and their constraint violations are evaluated using inexpensive constraint functions (line 6 to 7). We first select the feasible individuals and calculate the Euclidean distance between each offspring individual and each individual in the archive in the decision space. The offspring whose distance is less than the $Size_{niche}$ is deleted and then are merged into the archive (lines 8 to 10). When the population has more than N feasible solutions, individuals are selected according to the generation of the individual entering the population (lines 11 to 16). After the stopping criterion is met, the set of feasible solution archives is divided into N_{init} classes by the K-Means clustering algorithm, and one individual from each class is

Algorithm 1: Feasible Sampling Strategy

Input: $Size_{niche}$(threshold of Euclidean distance), Gen(maximum evolution generation), N(Feasible Sampling Strategy population size), N_{init}(output population size), FA(feasible archive), FP(feasible population), $problem$

Output: Pop_{init}

1 $pop \leftarrow LatinHyperCubeSampling(N, problem)$;
2 $gen \leftarrow 0$;
3 $FA \leftarrow SelectFeasibleInds(Pop)$;
4 $FP \leftarrow \phi$;
5 **while** $gen < Gen$ **do**
6 $\quad off \leftarrow$ Generate offspring based on pop by the operators of GA;
7 $\quad Evaluate(off, problem, 'CV')$;
8 $\quad off \leftarrow SelectFeasibleInds(off)$;
9 $\quad off \leftarrow DeleteCloseInds(FA, off, Size_{niche})$;
10 $\quad FA \leftarrow FA \cup off$;
11 $\quad FP \leftarrow SelectFeasibleInds(off \cup pop)$;
12 $\quad$ **if** $FP > N$ **then**
13 $\quad\quad pop \leftarrow FitnessSurvival(FP, 'gen', N)$
14 $\quad$ **else**
15 $\quad\quad pop \leftarrow FitnessSurvival(pop \cup off, 'CV', N)$
16 $\quad$ **end**
17 $\quad gen \leftarrow gen + 1$;
18 **end**
19 $clusters \leftarrow KMeansCluster(FA, N_{init})$;
20 $Pop_{init} \leftarrow RandomSelect(clusters)$;

randomly selected to form the initial population (lines 19 to 20).

B. Surrogate-ensemble Model

In this paper, the surrogate-ensemble model applied by the proposed SEACoEA is composed of RBF model and Kriging model. In addition, not only to balance between exploitation and exploration in the process of population evolution, but also to make full use of the advantages of Kriging model in the predicting uncertainty, the proposed SEACoEA applies the combination of RBF model and Kriging model to calculate the lower confidence bound (LCB) of each individual as its objective value. The i-th objective value of each individual is calculated as follows:

$$\hat{f}_i(\mathbf{x}) = \lambda_1 \hat{f}_i^{RBF}(\mathbf{x}) + \lambda_2 \hat{f}_i^{Kriging}(\mathbf{x}) - \gamma \hat{\sigma}_i(\mathbf{x}) \tag{6}$$

where $\hat{f}_i^{RBF}$ represents the i-th objective value predicted applying the RBF model; $\hat{f}_i^{Kriging}$ and $\hat{\sigma}_i$ represents the mean and variance of the i-th objective predicted applying the Kriging model; λ_1 and λ_2 represent the weights of $\hat{f}_i^{RBF}$ and $\hat{f}_i^{Kriging}$ respectively, and need to satisfy $\lambda_1 + \lambda_2 = 1$. γ is a trade-off constant of exploitation and exploration.

It is worth noting that, in the assisted optimization process using the surrogate-ensemble model, CCMO is used as a coevolutionary framework to solve ECMOPs and NSGA-II is used as an optimizer to evolve two populations. When the optimization reaches the maximum evolutionary generation, two populations are taken as output.

C. Infill Strategy

It is necessary to balance the relationship between exploitation and exploration, when selecting candidate solutions for expensive evaluation. To this end, in the assisted optimization process, the proposed LCB is used to calculate the objective value, which balances between exploitation and exploration during optimization. In addition, when selecting candidate solutions for expensive evaluation, the non-dominated solutions of two populations are divided into $N_{candidate}$ classes applying the K-means clustering algorithm, respectively, which can enhance the diversity of population. In order to further improve the exploration of the proposed algorithm, one of the non-dominated solutions in each class is randomly selected according to the crowding distance as candidate solutions, which may reduces the negative impact caused by the estimation error of the model.

IV. Experimental Comparison

In this section, the MW test suite [31] is adopted as test problems. The decision variable dimension of MW test suite is 15. The above problems are considered under the condition that the objectives are expensive and the constraints are inexpensive. Several state-of-the-art constrained multi-objective evolutionary algorithms for expensive problems, including IC-SA-NSGA-II [20], SA-NSGA-II [20], MOEA/D-EGO [32] , are employed. Since the proposed algorithm adopts the CCMO framework [28] to deal with CMOPs with expensive objectives and inexpensive constraints, CCMO is also employed as a comparison algorithm.

A. Experimental Setting

In the experiment, population size of each compared algorithm is set to 100, the maximum number of expensive evaluation is 600, and each algorithm runs 11 times separately. The initial number of individuals is $11n+25$ (n is the decision variable dimension), and 100 individuals are select as initial population. For the feasible sampling strategy in this paper, the initial population size is set to 500, and the maximum evolutionary generation is set to 100. The compared algorithms apply Latin Hypercube sampling method. For SEACoEA, λ_1, λ_2 and γ are set to 0.5, 0.5 and 3, respectively. Both the generation of surrogate model and the generation of CCMO-guide evolution are set to 20. The number of individuals updated is set to 10, in which the number of candidate solutions selected by $population1$ and $population2$ are set to 5 and 5, respectively. For the comparison algorithms, the default parameters of the original paper are used, except for the number of expensive evaluation, population size and the initial individual number. The code of IC-NSGA-II and SA-NSGA-II can be obtained from Julian Blank's personal homepage[1];

[1] https://julianblank.com/static/misc/pycheapconstr.zip

TABLE I
IGD INDICATOR OF CCMO, MOEA/D-EGO-CDP, SA-NSGA-II, IC-SA-NSGA-II AND SEACOEA. HIGHLIGHT THE BEST RESULT PER ROW "N/A" MEANS THAT NO FEASIBLE SOLUTION HAS BEEN FOUND "+", "−" AND "≈" INDICATE SIGNIFICANTLY BETTER, SIGNIFICANTLY WORSE AND STATISTICALLY SIMILAR COMPARED TO SEACOEA, RESPECTIVELY.

Problems	M	CCMO	MOEA/D-EGO-CDP	SA-NSGA-II	IC-SA-NSGA-II	SEACoEA
MW1	2	N/A	N/A	0.05993 (0.02363) −	0.04149 (0.00252) −	**0.02163 (0.00274)**
MW2	2	N/A	N/A	0.05604 (0.01073) +	**0.03816 (0.00334)** +	0.06762 (0.01032)
MW3	2	N/A	0.89008 (0.21726) −	0.03254 (0.02312) −	0.02097 (0.00390) −	**0.01332 (0.00124)**
MW4	3	N/A	N/A	0.11015 (0.01936) ≈	**0.07230 (0.00453)** +	0.09921 (0.00538)
MW5	2	N/A	N/A	0.31571 (0.02724) −	0.24447 (0.02071) −	**0.16660 (0.03335)**
MW6	2	N/A	N/A	0.53490 (0.16442) −	0.29538 (0.16933) ≈	**0.20654 (0.20555)**
MW7	2	N/A	0.52199 (0.15301) −	0.05020 (0.01100) −	0.11147 (0.15382) −	**0.02703 (0.00365)**
MW8	3	N/A	N/A	0.15068 (0.03956) ≈	**0.10051 (0.00442)** +	0.12402 (0.00539)
MW9	2	N/A	N/A	0.13350 (0.00809) −	0.10887 (0.01657) −	**0.08698 (0.01403)**
MW10	2	N/A	N/A	0.15905 (0.06021) −	0.07335 (0.02217) ≈	**0.07003 (0.01685)**
MW11	2	N/A	0.52677 (0.03172) −	0.47998 (0.16205) −	**0.20640 (0.15445)** ≈	0.27962 (0.19521)
MW12	2	N/A	N/A	0.18575 (0.01194) −	0.12395 (0.03400) −	**0.06560 (0.01603)**
MW13	2	N/A	N/A	0.17575 (0.00963) −	0.18000 (0.01463) −	**0.09509 (0.00291)**
MW14	3	N/A	N/A	0.69143 (0.12153) −	0.70182 (0.09645) −	**0.20658 (0.09023)**
+ / ≈ / −		0 / 0 / 0	0 / 0 / 3	1 / 2 / 11	3 / 3 / 8	

MOEA/D-EGO and CCMO are implemented by PlatEMO. The code can be obtained from PlatEMO's Github homepage[2].

B. Experimental Results

Table I shows the mean and variance of IGD values for CCMO, MOEA/D-EGO-CDP, SA-NSGA-II, IC-SA-NSGA-II and SEACoEA after 11 independent runs on MW test suite. The proposed SEACoEA outperforms the comparison algorithms, including IC-SA-NSGA-II, SA-NSGA-II, MOEA/D-EGO-CDP, CCMO in most MW problems, as shown in Table I. Table I also shows Wilcoxcon statistical test results. It can be observed that the proposed SEACoEA has significantly better performance than IC-SA-NSGA-II in 8 test problems and significantly better performance than SA-NSGA-II in 11 test problems. In addition, it is easy to find that the proposed SEACoEA is significantly better than MOEA/D-EGO-CDP in all the tested problems. To this end, it can be concluded that the proposed SEACoEA improves the search ability of CCMO to deal with expensive constrained multi-objective problems.

In addition, Fig. 2 shows the feasible non-dominated solutions of the proposed SEACoEA and the compared algorithms on MW1, MW3, MW7 and MW9 test problems, respectively. Fig. 2 clearly shows that the proposed SEACoEA has better convergence and diversity than the compared algorithms. Some possible reasons are as follows: (1) CCMO is applied to coevolve two populations, so that knowledge can be transferred between the two populations, which improves the search efficiency. (2) When selecting candidate solutions for expensive evaluation, feasible non-dominated solutions and infeasible non-dominated solutions are selected, which allows the surrogate-ensemble model to have better prediction accuracy not only in the feasible region, but also in the infeasible region, so that the population can maintain better diversity during the evolutionary process. (3) The surrogate-ensemble model is used to guide the population evolution, which can provide higher prediction accuracy and robustness than using only one surrogate model. In addition, the proposed LCB is used to calculate the objective value, which has a good balance between exploitation and exploration. (4) The proposed feasible sampling strategy allows the population to be initialized in the feasible regions, which improves the search efficiency.

[2]https://github.com/BIMK/PlatEMO

V. CONCLUSIONS

In this paper, a surrogate-ensemble assisted coevolutionary algorithm, named SEACoEA, is proposed to solve CMOPs with expensive objective and inexpensive constraints. The core idea of the proposed SEACoEA is to transfer the excellent search ability of coevolutionary algorithm in CMOPs to ECMOPs. SEACoEA applies the proposed feasible sampling strategy, surrogate-ensemble model and infill strategy combined with the CCMO framework to obtain Pareto solutions in a limited number of expensive evaluations. The experimental results show that the proposed SEACoEA has efficient searching ability in the CMOPs with expensive objective and inexpensive constraints. In other words, compared with other algorithms, the proposed SEACoEA has good convergence and diversity, which can obtain a set of Pareto solutions in CMOPs with expensive objective and inexpensive constraints. Based on the above comparative experimental results, several conclusions can be summarized as follows: (i) SEACoEA can search for the Pareto solution set of constrained multi-objective problem in a limited number of expensive evaluation, and has well convergence and diversity. (ii) Coevolution can be used to solve expensive constrained multi-objective problems. However, how to make populations cooperate more efficiently under expensive conditions is still a problem worth considering. Since a main feature of inexpensive constraint problems is that the Pareto solutions are usually on the boundaries of the constraints. How to combine the surrogate model to search non-dominated solutions on the constraint boundaries to assist the search of the original problem is a future work.

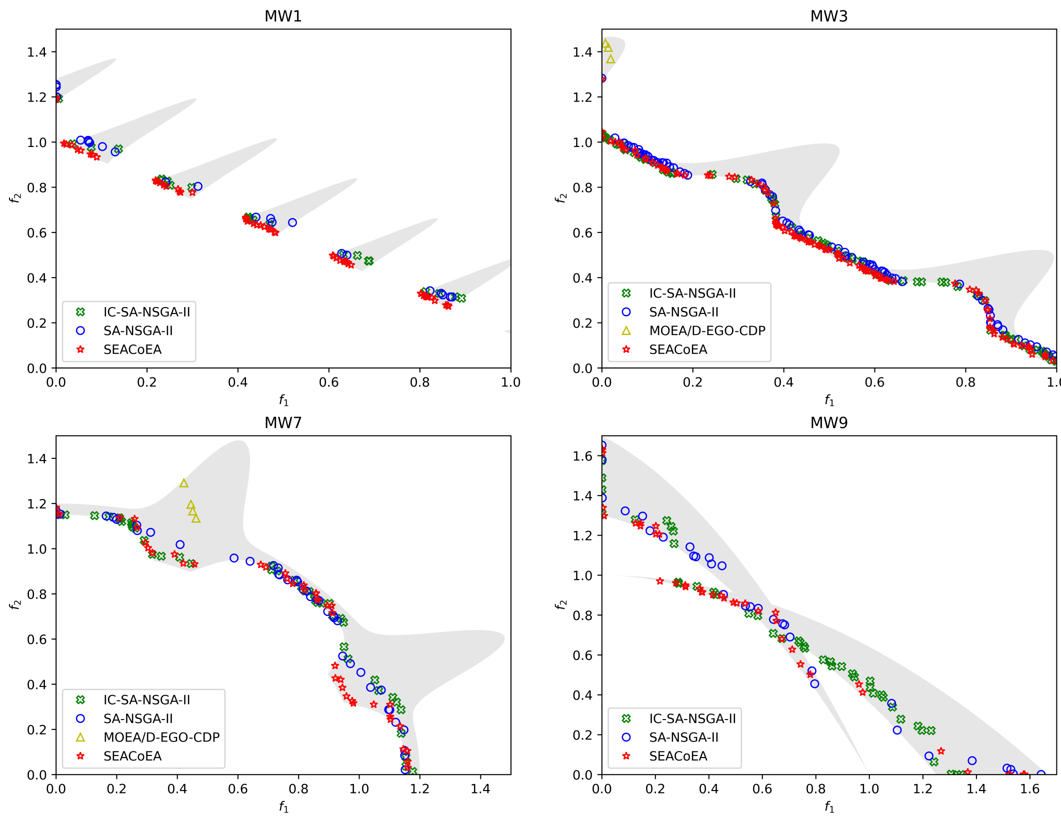

Fig. 2. Feasible and non-dominated solutions with median IGD value among 11 runs obtained by CCMO, MOEA/D-EGO-CDP, SA-NSGA-II, IC-SA-NSGA-II and SEACoEA on MW1, MW3, MW7 and MW9.

VI. Acknowledgement

This research was supported in part by National Key R&D Program of China (grant number 2021ZD0111501, 2021ZD0111502), the Key Laboratory of Digital Signal and Image Processing of Guangdong Province, the Key Laboratory of Intelligent Manufacturing Technology (Shantou University), Ministry of Education, the Science and Technology Planning Project of Guangdong Province of China (grant number 180917144960530), the Project of Educational Commission of Guangdong Province of China (grant number 2017KZDXM032), the State Key Lab of Digital Manufacturing Equipment & Technology (grant number DMETKF2019020), National Natural Science Foundation of China (grant number 62176147, 51907112, U2066212, 61961036, 62162054), STU Scientific Research Foundation for Talents (grant number NTF21001, NTF20009), Science and Technology Planning Project of Guangdong Province of China (grant number 2019A050520001, 2021A0505030072, 2022A1515110660, 2021A1515011709), and Science and Technology Special Funds Project of Guangdong Province of China (grant number STKJ2021176, STKJ2021019), Jiangxi"Double Thousand Plan" Project (JXSQ20210019).

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