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Study on the incorporation of PCA into EMO for high dimensional multi-objective problems

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***Abstract*—It has been known that the dimensionality reduction method is very effective for high dimensional (many design variable) problems in the field of evolutionary computation. Although there are proposed many approaches with this method for single-objective problems, the number of approaches with this method for multi-objective problems is very limited. In multi-objective optimisation, the desgin space to be explored is too large to reduce the number of dimension in the space appropriately. In this research, we focused on principal component analysis (PCA) as a simple dimensionality reduction method and investigated effective ways of incorporating this into evolutionary multi-objective optimization (EMO) algorithms. In this paper, we compared two original incorporated methods and verified the effect of different ways of incorporating; a straight-forward method and a more elaborated method. Because both of our methods are based on MOEA/D, we called these as MOEA/D-PCA and MOEA/D-Modified-PCA(MOEA/D-MPCA). Through applying these to some typical benchmark problems, we confirmed the effectiveness of MOEA/D-MPCA in comparison with the original MOEA/D and MOEA/D-PCA.**

***Index Terms*—evolutionary multi-objective optimization (EMO) ; PCA; dimensionality reduction; MOEA/D**

I. Introduction

Evolutionary Multi-objective Optimization (EMO) is one of the most active research areas in evolutionary computation, and various EMO algorithms have been proposed to date [1], [2].

On the other hand, the dimensionality reduction method has been very effective for high dimensional (many design variable) problems in this field. Although there are proposed many approaches with this method for single-objective optimization problems (SOOPs), the number of approaches with this method for multi-objective optimization problems (MOOPs) is very limited. There are some evolutionary multi-objective optimization (EMO) algorithms with dimensionality reduction method for reducing the dimension of objective space [3], [4], but approaches for reducing that of design valuable space.

The reason for this is that the search space of MOOPs is larger than that of SOOPs and it is very difficult to effectively compress a high dimensional search space into a lower dimensional space.

In this research, we focused on principal component analysis (PCA) as a simple dimensionality reduction method and investigated effective ways of incorporating this into EMO algorithms.

When to incorporate PCA into EMO, it is necessary to invent ways to overcome the difficulties inherent in MOOPs. Therefore, we implemented two original EMO methods with PCA in this paper; a straight-forward method and a more elaborated method. Because both of our methods are based on MOEA/D, we called these as MOEA/D-PCA and MOEA/D-Modified-PCA(MOEA/D-MPCA). MOEA/D-MPCA has three particular improvements compared to simple version (MOEA/D-PCA).

In order to verify the usefulness of incorporating PCA into EMO, we applied these to the WFG test suites and compared the performance of original MOEA/D, MOEA/D-PCA, and MOEA/D-MPCA.

II. Related works

In this section, we describes the elements of the proposed method and previous studies. : MOEA/D, a typical EMO algorithm, PCA, a classical statistical method, and C-PCA-NSGA-Ⅱ [3], a previous studies incorporating PCA in EMO.

A. MOEA/D

MOEA/D is an EMO algorithm proposed by Zhang et al. in 2007 [5]. Fig. 1 shows the general concept of MOEA/D. In the Fig. 1, F is the objective function, x is the population, g is the weight vector, and z is the reference point. It is a decomposition-based method that decomposes a multi-objective optimization problem into multiple single-objective optimization problems using a scalarization function. There are some different subspecies, like MOEA/D-DU [6], MOEA/D-DD [7] and so on.

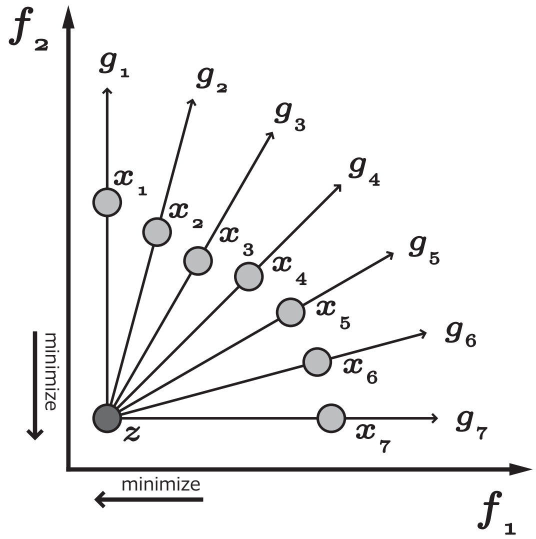

Fig. 1: Concept of MOEA/D

B. PCA

PCA is a typical linear dimensionality compression method. It has been used in various fields for feature analysis and visualization of data. PCA finds the direction with the maximum variance of the data projected on the axes as the first principal component, and obtains the second and third principal component axes with the maximum variance for the residuals. This enables dimensional compression that preserves variance in a multidimensional data space.

*C. C-PCA-NSGA-*Ⅱ

C-PCA-NSGA-Ⅱ incorporates Correntropy PCA(C-PCA) [8] for NSGA [9] and simplifies the objective function space by reducing the dimension of PCA. This approach uses dimensionality reduction for reducing the dimension of the design valuable space, but dimensionality reduction of the objective space is not mentioned.

III. Proposal Method

In this paper, we proposed two different approaches to investigate the usefulness of PCA utilization in EMO. These approaches are named " MOEA/D Principal Component Analysis (MOEA/D-PCA)", and MOEA/D Modified Principal Component Analysis(MOEA/D-MPCA)" because it is based on MOEA/D.

This is because the search space to be explored in the multiobjective problems is so distributed over a large area and it is difficult to carry out appropriate dimensionality reduction of the space.

MOEA/D-PCA was designed as a simple way to incorporate PCA into MOEA/D. Therefore, this method applies PCA to the population of each MOEA/D subproblem and generate new solutions on the principal component space without any complicated operations.

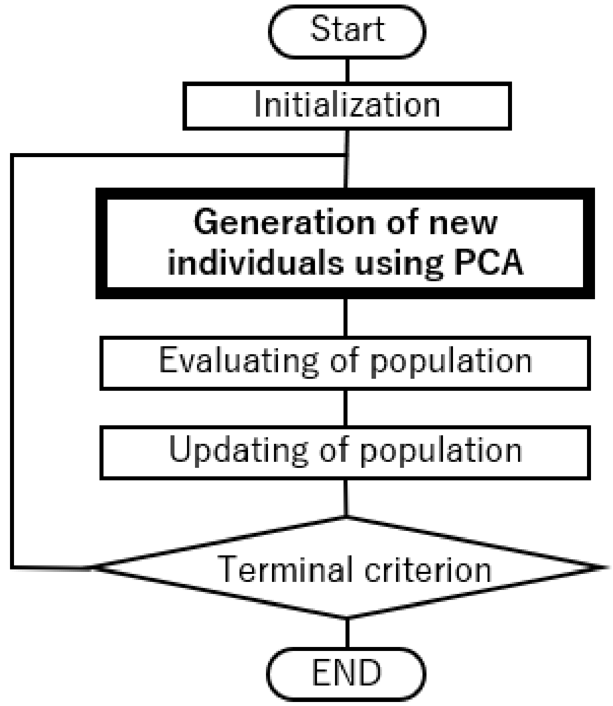

Fig. 2: The flow of MOEA/D-PCA

MOEA/D-MPCA, on the other hand, focused on making PCA work effectively on EMO. Compared to MOEA/D-PCA, MOEA/D-MPCA has some improvements such as the use of evolutionary differences and past information. In other words, MOEA/D-MPCA is a more EMO-adapted version of MOEA/D-PCA.

In the following, we described the flow of MOEA/D-PCA firstly, and then the flow of MOEA/D-MPCA, which is an improved version of MOEA/D-PCA.

A. MOEA/D-PCA

MOEA/D-PCA is based on MOEA/D. The most important point of MOEA/D-PCA is that new solutions are generated in a space whose dimension is reduced by PCA. Since dimensionality compression using PCA is more effective for higher dimensional problems, MOEA/D-PCA is expected to be more effective for higher dimensional problems. The flow of MOEA/D-PCA is shown in Fig. 2.

The bold frame in the Fig. 2 shows the characteristic parts of MOEA/D-PCA compared to the original MOEA/D. In the following, we describe the parts enclosed by the bold frame in detail.

Generation of new individuals using PCA: The new solution generation using PCA is performed for each weight vector $\boldsymbol{\lambda}_1, \ldots, \boldsymbol{\lambda}_N$ as in MOEA/D.

The solution $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_T$ corresponding to each of the T neighborhoods of $\boldsymbol{B}(i) = \{i_1, \ldots, i_T\}$ is analyzed using PCA to reduce its dimension to generate a simplified design variable space (hereinafter referred to as PCA space), and the population is also converted to a solution adapted to the PCA space.

Then, a new solution is generated in the PCA space, and finally it is converted back to the solution in the original space for evaluation.

We show procedure for generating a new solution in PCA space as below.

Step.1 Do PCA
The eigenvalues and eigenvectors are obtained from the $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_T$ corresponding to each of the T neighborhoods $\boldsymbol{B}(i) = \{i_1, \ldots, i_T\}$ by PCA. The principal components are obtained so that the cumulative contribution ratio $R > 0.8$.

Step.2 Indivisdals conversion
Transform $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_T$ into the solution $\boldsymbol{p}_1, \ldots, \boldsymbol{p}_T$ in PCA space from the transformation matrix obtained by PCA in Step 1.

Step.3 Crossover and Mutation
Generates a new solution $\boldsymbol{p}_{new}$ similar to MOEA/D.

Step.4 inversion of Individuals
Find the transpose matrix of the transformation matrix obtained by PCA in Step.2. Transform $\boldsymbol{p}_1, \ldots, \boldsymbol{p}_T, \boldsymbol{p}_{new}$ to the solution $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_T, \boldsymbol{x}_{new}$ in the original space.

B. MOEA/D-MPCA

MOEA/D-MPCA is a method to improve the problems of MOEA/D-PCA and to make PCA more adapted to EMO.

One of important features in MOEA/D-MPCA is to use the information of evolutionary difference vector from past solutions when to generate new solutions. Therefore, MOEA/D-MPCA tries to generate new solutions in the direction derived from past information.

On the other hand, for problems where the PCA spatial transformation does not work well, a normal MOEA/D mechanism is used again to ensure at least MOEA/D results.

The flow of MOEA/D-MPCA is shown in Fig. 3. The bold frame in the figure shows the characteristic parts of MOEA/D-MPCA compared to MOEA/D-PCA before the improvement. In the following, we describe the parts enclosed by the bold frame in detail.

Collect data: In MOEA/D-PCA, PCA is applied from the beginning of the search using only the neighboring solutions of the generation. this approach had problems which lead to a poor accuracy in finding axes directly related to changes in evaluation values.

Therefore, MOEA/D-MPCA accumulates $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_T$ solutions corresponding to each of the T neighboring $\boldsymbol{B}(i) = \{i_1, \ldots, i_T\}$ without allowing duplication in each generation, and PCA is performed in a state in which the trend of solutions can be easily grasped to some extent.

In this paper, the data accumulation interval is up to 3000 evaluations.

Decide whether to use PCA: Since PCA is a linear projection, it may be effective locally but counterproductive overall, depending on the problem characteristics. Although the search

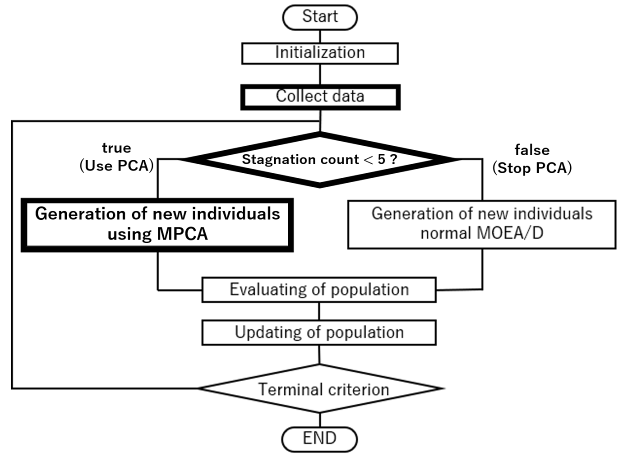

Fig. 3: The flow of MOEA/D-MPCA

policy is defined by the evolutionary difference vector, we decided to stop the use of PCA when the search in the PCA space still fails to proceed. In this paper, we revert to the normal MOEA/D solution generation mechanism when the update of solution fails a certain number of times.

This process makes it possible to obtain a solution equivalent to that of regular MOEA/D even for problem characteristics where PCA does not work well.

Generation of new individuals using MPCA: The concept of the evolutionary difference vector is shown in Fig. 4. The evolutionary difference vector represents the evolutionary process of each solution in the population. Therefore, by keeping and accumulating the differences at each solution update, it is possible to get a rough idea of the direction in which the solution will improve in terms of evaluation value. In MPCA, new solutions are generated under the influence of the direction calculated by the evolutionary differences of the last five times. For this reason, MPCA can be expected to generate new solutions in the more promising direction.

We show procedure for generating a new solution using MOEA/D-MPCA as below. The parts that do not differ from MOEA/D-PCA are omitted for the sake of brevity.

Step.1 Do PCA
Same as MOEA/D-PCA.

Step.2 Indivisdals conversion
During the transformation to the solution corresponding to the PCA space, the evolutionary difference vector held by each solution is also transformed using the transformation matrix.

Step.3 Crossover and Mutation
A new solution $\boldsymbol{p}_{new}$ similar to MOEA/D is generated, and the positions of the $\boldsymbol{p}_{new}$ are corrected in the vector direction that bisects the angle between the evolutionary difference vector and the vector in the direction of the new solution.

Step.4 inversion of Individuals
Inverse transformation to the solution corresponding to the original space.

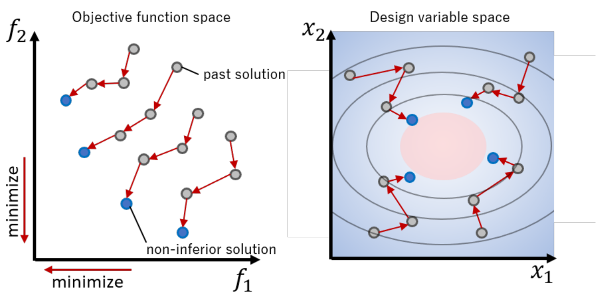

Fig. 4: Concept of the evolutionary difference vector

In this process, the evolution difference vector held by each solution is also transformed using the transpose matrix of the transformation matrix.

MOEA/D-MPCA is expected to demonstrate the effectiveness of PCA utilization in EMO by incorporating PCA into EMO in an ingenious way, rather than by incorporating PCA into EMO in an unplanned way as MOEA/D-PCA does.

IV. Experiments

To investigate the usefulness of utilizing PCA in EMO, we applied it to the WFG test suites and compared the performance of three approaches, MOEA/D, MOEA/D-PCA and MOEA/D-MPCA. In this experience, we used our proposal MOEA/D-ADAPT [10] as simple MOEA/D, and MOEA/D-PCA and MOEA/D-MPCA are based on this MOEA/D-ADAPT. In this experiment, the average of 50 trials (mean) was used as the result of each algorithm.

In this section, we present the instances, the measuring methods, the setting parameters and the results of experiments.

A. Instances

We used WFG test suites [11] as instances. WFG has been widely used as typical test problems and can change the number of objectives and variables optionally.

In this experiments, we set position parameter $k = 2(M-1)$ and distance parameter $l = n-k$. (M is number of objectives, n is number of design variables) In addition, the upper bound of variables of WFG is not same, so we normalized the variables in all test problems.

B. Measuring Methods

We used inverted generational distance plus (IGD+) [12] and hypervolume (HV) [13] as performance indicators. We show the details of these as below.

IGD+: IGD+ is the distance between solutions and Pareto solutions (Pareto front). Lower value of IGD+ means that solutions is closer to Pareto front. In these experiments, we used the data of jMetal Web Site [14] as the sampling data of Pareto front.

HV: HV is the size of the objective space dominated by solutions. Therefor HV value can be used as a comprehensive indicator considering “accuracy”,“width”, and “uniformity”. In these experiments, we set the reference point r of HV to $r = (3, 5, 7)$.

TABLE I: Used parameters of MOEA/D-MPCA

Parameters	Values
#Objectives (M)	3
#Design variables (n)	$10, 50, 100$
Neighborhood size (T)	20
Division Parameter (H)	19
Population size (N)	200
Terminal criteria (#evaluate)	50000
Cumulative contribution rate (R)	0.8
Stagnation count	5
Data collection limit	3000
CX operation	MOEA/D-DE
Selection method	MOEA/D-DU

C. Settings Parameters

The used parameters of MOEA/D-MPCA are shown in Table I. In MOEA/D for these experiments, we used MOEA/D-DE as CX and MOEA/D-DU as selection method. From the results of pre-examination, In this experiment, Stagnation count was determined five times.

D. Results of Experiments

The mean results of comparative experiments are shown in Table II to Table VII. In addition, Fig. 5 is the transition graph of IGD+ in the experiments set $n = 100$.

These results show that PCA in EMO is highly dependent on the characteristics of the problem to be solved. The MOEA/D-PCA results show that simply incorporating PCA without any effort will only interfere with the search in most problems. However, Fig. 5b, Fig. 5f and Fig. 5i show an advantage in the early stage of the search, although the final result is inferior to MOEA/D. Especially, In Fig. 5c, MOEA/D-PCA outperforms MOEA/D throughout the search. This can be considered as an example that the dimensionality reduction by PCA worked effectively and reduced the difficulty of the search.

In addition, the results of MOEA/D-MPCA with high dimensionality show that MOEA/D-MPCA is able to utilize PCA very effectively compared to MOEA/D-PCA. In particular, MOEA/D-MPCA succeeded in improving the performance of MOEA/D in Fig. 5b, Fig. 5c, and Fig. 5d. In other problems, if there is no prospect of utilizing PCA, the Search mechanism reverts to the normal MOEA/D mechanism, and thus the performance of MOEA/D is at least guaranteed.

The use of PCA in EMO was confirmed to have a certain usefulness for high-dimensional problems, although it depends on the problem characteristics. On the other hand, the usefulness of PCA was not confirmed for low-dimensional problems.

V. Conclusion

In this paper, we presented new EMO algorithms ”MOEA/D-Principal Component Analysis (MOEA/D-PCA)” and ”MOEA/D-Modified Principal Component Analysis (MOEA/D-MPCA)”, which incorporate PCA into existing EMO algorithms for complessing the design variable space. To verify the usefulness of utilizing PCA in EMO, and compared the experimental results.

Compared to MOEA/D-PCA, which applies PCA to EMO without any special modifications, MOEA/D-MPCA was able

TABLE II: The result IGD+ of $n = 10$ experiments

	MOEA/D	MOEA/D -PCA	MOEA/D -MPCA
WFG1	**1.39658**	2.1571	1.39948
WFG2	**0.0207679**	0.257217	0.0289252
WFG3	**0.0132787**	0.296685	0.013828
WFG4	**0.0897082**	0.213817	0.101988
WFG5	**0.0865915**	0.445136	0.0866219
WFG6	**0.0409027**	0.204688	0.0453014
WFG7	**0.0364459**	0.471644	0.0470396
WFG8	**0.216151**	0.601756	0.228632
WFG9	**0.0400011**	0.32141	0.0472828

TABLE III: The result HV of $n = 10$ experiments

	MOEA/D	MOEA/D -PCA	MOEA/D -MPCA
WFG1	**47.3914**	14.2205	47.6154
WFG2	**100.977**	89.1021	98.6507
WFG3	**76.5368**	67.9191	75.3547
WFG4	**75.2455**	60.5634	74.321
WFG5	**74.166**	52.2529	73.9993
WFG6	**78.0178**	68.3856	77.6098
WFG7	**78.1116**	51.7328	75.3754
WFG8	**66.7852**	47.2925	65.5903
WFG9	**74.8656**	57.6064	72.0348

TABLE IV: The result IGD+ of $n = 50$ experiments

	MOEA/D	MOEA/D -PCA	MOEA/D -MPCA
WFG1	**1.43945**	2.1637	1.44886
WFG2	0.379568	0.423202	**0.336802**
WFG3	0.429281	0.432447	**0.410673**
WFG4	**0.239026**	0.319317	0.255724
WFG5	0.159368	0.723489	**0.158372**
WFG6	**0.191935**	0.353567	0.192982
WFG7	**0.360545**	0.542728	0.495556
WFG8	**0.294971**	0.731918	0.301775
WFG9	**0.191811**	0.329119	0.191862

TABLE V: The result HV of $n = 50$ experiments

	MOEA/D	MOEA/D -PCA	MOEA/D -MPCA
WFG1	**46.3756**	13.7783	46.1397
WFG2	82.227	81.3778	**82.9524**
WFG3	65.2173	63.7841	**65.2189**
WFG4	**66.787**	57.4757	64.7576
WFG5	70.2031	42.6785	**70.7431**
WFG6	**70.6636**	60.4425	70.6131
WFG7	**61.344**	51.8046	55.1092
WFG8	**64.6506**	43.4613	63.0644
WFG9	**66.7011**	58.0228	64.2466

TABLE VI: The result IGD+ of $n = 100$ experiments

	MOEA/D	MOEA/D -PCA	MOEA/D -MPCA
WFG1	1.44312	2.15728	**1.44293**
WFG2	0.465014	0.469031	**0.435356**
WFG3	0.52332	0.490224	**0.484492**
WFG4	**0.279716**	0.349998	0.289949
WFG5	0.194593	0.744537	**0.182647**
WFG6	0.249973	0.431449	**0.218696**
WFG7	**0.432498**	0.595191	0.435258
WFG8	**0.329159**	0.766499	0.337661
WFG9	0.25475	0.331815	**0.253849**

TABLE VII: The result HV of $n = 100$ experiments

	MOEA/D	MOEA/D -PCA	MOEA/D -MPCA
WFG1	**46.3168**	13.9486	46.1232
WFG2	78.2217	79.5583	**80.2103**
WFG3	62.7494	62.6728	**62.8701**
WFG4	**64.6846**	56.5415	61.9913
WFG5	68.5813	42.0285	**69.4941**
WFG6	66.6415	57.4627	**68.221**
WFG7	**58.3208**	49.4539	55.1097
WFG8	**63.5722**	42.1226	59.9801
WFG9	**63.8932**	57.6849	63.3221

to improve search efficiency by utilizing past solution information and using evolutionary difference vectors in PCA space. Furthermore, even if PCA does not work effectively due to problem characteristics, it can detect search stagnation and return to the base method, guaranteeing at least equivalent or better performance. By seeking ways to incorporate effective PCA into EMO as in this paper, we aim to improve the efficiency of search, especially for high-dimensional problems.

Comparison of MOEA/D, MOEA/D-PCA and MOEA/D-MPCA shows that MOEA/D-MPCA performs better than other EMO algorithms on high-dimensional problems, although it has some problems such as PCA does not work well on low-dimensional problems and is affected by the problem characteristics.

Therefore, it can be said that the use of PCA in EMO has great potential, although there are many problems to be considered.

VI. Acknowledgement

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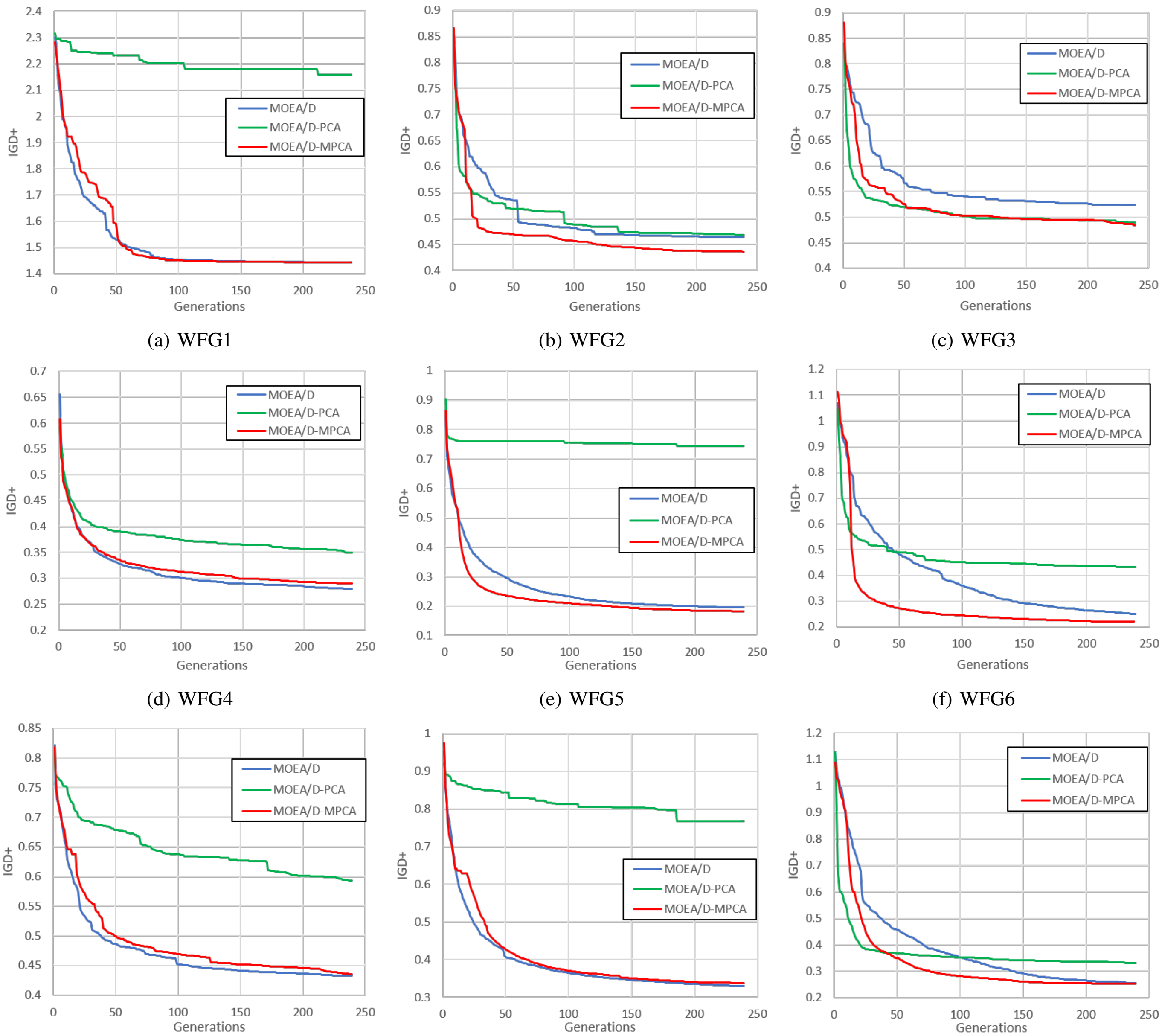

(a) WFG1 (b) WFG2 (c) WFG3

(d) WFG4 (e) WFG5 (f) WFG6

(g) WFG7 (h) WFG8 (i) WFG9

Fig. 5: Transitions of IGD+

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