# A Proposal of Visualization of Multi-Objective Pareto Solutions -Development of Mining Technique for Solutions-

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Abstract—Recently, the rapid progresses of computers introduce evolutionary computations to next step, which is the demand for the variety of Pareto solutions in multi-objective optimization problems. We can calculate a large amount of Pareto solutions in a short time. However, it is difficult to use the acquired Pareto solutions effectively, because the Pareto solutions have multi-dimension of fitness values. This study tries to develop "Mining of solutions" technique with visualization. This paper proposes a visualizing method for Pareto solutions which have multi-objective fitness values. The proposed method enables us to grasp the distributed structure of Pareto solutions and clarify the relationship among multi-objective fitness values. This paper shows that the visualized data enables us to interpret the characteristics of Pareto solutions through experimental result.

## I. INTRODUCTION

**E** VOLUTIONARY Computations (ECs) are effective methods for optimization problems, and many researches and applications of ECs have been reported [1], [2], [3], [4], [5]. ECs have been required to search "better" solutions "faster" than other methods such as random search. On the other hand, the rapid progress of computers has been introducing evolutionary computations to next step, which is the demand for "more variety of Pareto solutions" in multi-objective optimization problems [6]. Fast-evolving and rapidly advancing of computer performance enable us to cal-

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Daisuke Yamashiro is with the Department of Computational Science and Engineering, Nagoya University, Furo-cho, Chikusa-ku, Nagoya, 464-8603, JAPAN (phone: +81-52-789-2793; fax: +81-52-789-3166; email: daisuke@cmplx.cse.nagoya-u.ac.jp).

Takeshi Furuhashi is with the Professor of Department of Computational Science and Engineering, Nagoya University, Furo-cho, Chikusa-ku, Nagoya, 464-8603, JAPAN (email: furuhashi@cse.nagoya-u.ac.jp). culate a large amount of candidates of solutions (Pareto solutions) in a short time. Non Dominated Sorting Algorithm-II (NSGA-II) [7] is one of the most effective methods to search Pareto solutions in Multi-Objective Optimization Problems. When we applied NSGA-II to a Nurse Scheduling Problem (NSP) [8] with 12 objective functions, approximately 5,000-10,000 Pareto solutions could be acquired in a trial.

A huge amount of stored data by IT technology has strongly needed and generated Data Mining techniques, in the same way, the demand for the techniques to analyze or show the acquired a lot of Pareto solutions with multidimensional fitness values effectively for users has been growing. This paper calls these techniques "Mining of solutions". This study aims to develop the technique of mining of solutions and employs the approach of visualization of Pareto solutions as one of the techniques. The visualization supports the interpretation of Pareto solutions having multidimensional fitness values easily and showing them to users effectively in Multi-Objective Optimization Problems.

Obayashi et al. have reported the visualization method of the Pareto solutions using Self Organizing Map (SOM) [9]. We have also proposed the visualization method of search process using SOM to grasp the effect of genetic operation in Genetic Algorithm (GA) [10]. SOM is one of the nonlinear mapping methods and it can generate a visible space in consideration of the distances among clusters or data. These nonlinear visualization methods are effective to grasp the similarities or the distribution of data such as relative distances among data. However, the generated map shows only the distance information of data, and it is difficult to interpret the characteristics of data[11].

This paper applys the visualization method using Fuzzy C-Means (FCM) and Fuzzy Multiple Discriminant Analysis (FMDA) proposed by Yamamoto et al. [12]. It employs

the linear combinations of input variables to reduce the dimensionality and visualize Pareto solutions. FCM is used for the clustering of Pareto solutions in the original dimensional space. FMDA is an extended method of the Multiple Discriminant Analysis (MDA) to deal with fuzzy clusters. The projection axes obtained as linear combinations of input variables are identified by FMDA, and they generate visible space. The proposed method makes the interpretation or analysis of Pareto solutions easier such as the distributed structures or similarities of Pareto solutions in multi-dimensional space, the relationships among the objective functions and the characteristics of the clusters through the meaning of projection axes. This method can also support decisionmaking for users such as selection of the acquired Pareto solutions by visualized result. In addition, this method can also give the information of search process such as the effect of genetic operations and the change of the distribution of Pareto solutions. This paper applies the proposed method to the Pareto solutions of NSP acquired by NSGA-II and investigates the effectiveness of this method.

This paper is organized as follows: Chapter 2 describes the proposed visualization method, chapter 3 explains the applied NSP, chapter 4 shows the experimental results and investigation and this paper concludes in chapter 5.

# II. VISUALIZATION METHOD

The flow of the proposed method is as follows:

- Step 1: Generating Pareto solutions by a Multi-Objective EC method
- Step 2: Selection of variables (objective functions)
- Step 3: Clustering Pareto solutions in multi-dimensional (fitness) space by Fuzzy C-Means (FCM)
- Step 4: Identification of projection axes and reduction of dimensionality by Fuzzy Multiple Dicriminant Analysis (FMDA)
- Step 5: Projection and visualization of Pareto solutions onto visible space consisting of the projection axes

First, the proposed method generates the candidates of solutions acquired by EC method such as NSGA-II and selects the variables used for the visualization from the objective functions. If the variance of the fitness value of a certain objective function in Pareto solutions is almost 0 or very small, it is regarded that it has few characteristics and the objective function is eliminated from the input variables for visualization. Second, FCM is applied to the candidates of solutions in order to identify clusters and grasp the distributed structure of Pareto solutions in multi-dimensional fitness space. FCM is a representive fuzzy clustering method. FCM, first, the preliminarily assigned  $N_C$  centers of clusters are initialized. Next,  $u_{ik}$ , degree of belonging to each *i* cluster are calculated by (1).

$$u_{ik} = \left[\sum_{j=1}^{N_C} \left(\frac{\|x_k - a_i\|^2}{\|x_k - a_j\|^2}\right)^{1/m_f - 1}\right]^{-1} \tag{1}$$

where  $m_f$  is a fuzziness parameter,  $x_k$  is  $k^{th}$  candidate of solutions ( $x_k = (x_{k1}, x_{k2}, \dots, x_{kP})$ ), P is the number of selected objective functions and each element means the fitness value of each objective function) and  $a_i$  means the vector of each cluster center.

The equation to update each cluster center  $a_i$  is as follows.

$$a_{i}^{(t+1)} = \frac{\sum_{k=1}^{N_{D}} \mu_{ik}^{(t)} x_{k}}{\sum_{k=1}^{N_{D}} \mu_{ik}^{(t)}}$$
(2)

The (t) in this equation represents the number of iterations and the  $N_D$  represents the number of the acquired candidates of solutions. In many cases, the fuzziness parameter  $m_f$ employs  $m_f = 2$  by convention, then this paper also employs  $m_f=2$ .

FCM generates clusters with repeating calculation of degree of belonging by equation(1) and updating each cluster center by equation (2), where the sum of degree of belonging to each cluster  $(\sum_{i=1}^{N_C} u_{ik} = 1)$ .

After the clustering by FCM, projection axes are identified by FMDA to reduce the dimensionality. The Projection axes are obtained as linear combinations of input variables and the number of projection axes is at most three as premises for visualization. This visualization method identifies projection axes which maximize the distances among the acquired clusters by FCM. FMDA is an extended method of MDA to deal with fuzzy clusters, and it can identify the projection axes to maximize the ratio between within-class scatter and between-class scatter in visible space. The within-class scatter matrix  $S_B$  and between-class scatter  $S_W$  in FMDA are as follows.

$$S_B = \sum_{i=1}^{N_C} \sum_{k=1}^{N_D} \mu_{ik} (m_i - v) (m_i - v)^t$$
(3)

$$S_W = \sum_{i=1}^{N_C} \sum_{k=1}^{N_D} \mu_{ik} (x_k - m_i) (x_k - m_i)^t$$
(4)

k=1

$$m_i = \frac{\sum_{k=1}^{N_D} \mu_{ik} x_k}{\sum_{k=1}^{N_D} \mu_{ik}} \tag{5}$$

$$v = \frac{1}{N_D} \sum_{i=1}^{N_D} x_k$$
 (6)

 $m_i$  represents the average of cluster centers in multidimensional fitness space and v represents the average vectors of fitness values in all candidates of solutions. The equations (3)-(6) are calculated with  $\mu_{ik}$  identified by FCM. And when  $\mu_{ik}$  is  $\{0, 1\}$ , the equations (3)-(6) correspond to the equations of MDA.

Using  $S_W$  and  $S_B$ , the discriminant is derived by solving a generalized eigenvalue problem expressed as

$$S_B w_l = \lambda_l S_W w_l. \tag{7}$$

The eigen vectors of  $S_W^{-1}S_B$  are the obtained projection axes in this method (where  $w_l$  is coefficient vectors of  $l^{th}$ projection axis). Since the  $S_W^{-1}S_B$  is an asymmetric matrix, the acquired projection axes are non-orthogonal to each other. The eigen values acquired by FMDA are the criterions for the proper number of dimensionality. The number of projection axes should be maximum three for the visualization. It should be noted that the FMDA does not guarantee that the proper projection axes for visualization are always acquired.

The projection axes  $\xi_l$  which generate visible space can be acquired by the obtained w.

$$\xi_l = w_l^t x = w_{l1} x_1 + w_{l2} x_2 \dots + w_{lP} x_P$$

$$(l = 1, 2, 3)$$
(8)

Through the above processes, the Pareto solutions are projected onto the visible space identified projection axes.

## **III. NURSE SCHEDULING PROBLEM**

								D	ate									
Skill	Name	1	2	3	4	5	6	7	8	9	10	11	12	13	14	D	Ν	М
Α	Staff A	Ν	Ν		Ν	Ν	М	Ν		D	D	М	Ν		D	3	6	2
Α	Staff B		D	D	Μ	D	D	М	Ν	Μ			D	Μ	Ν	5	2	4
Α	Staff C		D	D	Μ		Ν		D	D	Μ		Ν	D	D	6	2	2
В	Staff D	D	М		D	Μ	Ν	D		Ν	Ν	D	Μ		D	5	2	3
В	Staff E	D	D	М		Ν	D	D	М		D	D		Ν	Ν	6	3	2
В	Staff F	D	D	М	Ν	Ν		D	D	Μ		Ν	D	D	Μ	6	3	3
В	Staff G	Ν		D	D	Μ		Ν	D	D	Μ	Ν	D	D	Μ	6	3	3
С	Staff H	D	М	D	Ν		D	D	М		Ν	D	D	Μ	Ν	6	3	3
С	Staff I	М		Ν	D	D	М		Ν	D	D	М		D		5	2	3
С	Staff J	М	Ν	D		D	D	М		Ν	D	D	Μ	Ν	D	6	3	3
	D	4	4	4	3	3	4	4	3	4	4	4	4	4	4			
	M	2	2	2	2	2	2	2	2	2	2	2	2	2	2			
	N	2	2	1	3	3	2	2	2	2	2	2	2	2	3			

Fig. 1. Example of Nurse Scheduling Table

This chapter explains NSP, which is one of the actual multi-objective optimization problems. The authors have tried to put nurse scheduling support system to practical use and studied what kind of genetic operators and the parameters are most suitable for NSP [8]. The nurse schedule is updated by a nurse-in-chief of each department in every month. Nurse scheduling has taken much labor. A sample of nurse schedule is shown in Fig. 1. In this schedule, one of

three working patterns is allocated to each nurse (Staff-A to Staff-J). This schedule is a portion of one-month schedule. (In the experiment of this paper, one-month schedule of 26 nurses is employed.) The symbol D denotes day shift (AM 8:00 - PM4:00), N is night shift (PM4:00 - AM0:00), and M is midnight shift (AM0:00 - AM8:00). A box without any symbol means a day off. In the three rows at the bottom of the schedule, the allocated numbers of staff in each shift is shown. The leftmost column describes nurse's skill level. The skill level A means that he/she is an expert in nursing. The skill level C means that he/she is a fresh person, and B is in the middle of A and C. The three rightmost columns describe the allocated days to each shift to each nurse. There are many constraints on this scheduling. One of them is the series of shifts for every nurse. An example of prohibited pattern is to allocate a midnight shift right after the day off. Another constraint is that "One or more expert must be allocated at every midnight shift". NSP has many objective functions such as prohibition work patterns, balances among nurses' teams, fairness of holiday and so on.

There are 12 objective functions. That is, NSP is one of the multi-objective optimization problems whose objective function are their constraints. The objective functions of NSP employed in this paper are as follows:

- The number of requisite nurses in each shift per day
- · Level of requisite nurses in each shift per day
- The number of requisite nurses in each team per day
- Established prohibited working patterns
- · Established compromised working patterns
- Fairness of the number of working times on night or midnight shifts among nurses
- · Fairness of the number of holidays among nurses
- Fairness of the number of successive holidays among nurses
- The prescript number of working times per month on night or midnight shifts in each nurse (within 8times) (Note that the number of working times on night shift is between 3 and 5 times and that of midnight is 3 or 4 times)
- The prescript number of holidays per month in each nurse (more than 7 holidays)
- Successive holidays Saturday and Sunday in each nurse (one or more times per month)
- Successive holidays in each nurse (one or more times per month)

The number of violations in each objective function as described above is calculated on each candidate of solutions. The number of violations is employed as the fitness value of each objective function.

## IV. EXPERIMENT

This chapter shows the visualization results of the acquired Pareto solutions and discusses them. NSGA-II through 100,000 generations was applied to NSP.

### A. Identification of projection axes

First, this subsection shows the result of the variable selection as the step 2 of the proposed method. The variance of the fitness value on "the number of requisite nurses in each shift per day" was very small. And the variances of the objective functions on "fairness of the number of successive holidays among nurses", "the prescript number of holidays per month in each nurse", "successive holidays Saturday and Sunday in each nurse" and "successive holidays in each nurse" in the acquired Pareto solutions were almost 0. Then these objective functions were eliminated from the input variables for visualization. This experiment employs 7 objective functions and visualizes them. The employed objective functions are as follows:

- $Obj_1$ :Level of requisite nurses in each shift per day
- *Obj*<sub>2</sub>:The number of requisite nurses in each team per day
- *Obj*<sub>3</sub>:Established prohibited working patterns
- *Obj*<sub>4</sub>:Established compromised working patterns
- Obj<sub>5</sub>:Fairness of the number of working times on night or midnight shifts among nurses
- Obj<sub>6</sub>:Fairness of the number of holidays among nurses
- *Obj<sub>7</sub>*:The prescript number of working times per month on night or midnight shifts in each nurse (within 8times)

The number of clusters  $N_C$  was 5, which was decided based on an index of the ratio between within-class scatter and between-class scatter. Table 1 shows the acquired eigen values and eigen vectors (coefficient of projection axes  $w_l$ ) by FMDA.

Table 1 shows that the sum of the eigen values on the first and second projection axes was more than 90% in all eigen values. It means that the visible space using the first and second projection axes (2 dimensional space) can keep approximately 90% of the data structure in the multi-dimensional space.

The eigen vectors in table1 shows that the first projection axis was heavily affected by  $Obj_3$ ,  $Obj_5$ ,  $Obj_7$  and the second projection axis was by  $Obj_1$ ,  $Obj_2$ ,  $Obj_5$ . These results enabled us to label the first axis as "the violation axis in terms of the prohibited working pattern and night/midnight shift" and the second axis as "the violation axis in terms of the number of requisite nurses and fairness of the number of working times on night/midnight shift". In addition, the coefficients of  $Obj_3$ ,  $Obj_5$  and  $Obj_7$  on the first projection axis shows negative values. It means that the bigger the value



Fig. 2. Visualization Result at the  $100,000^{th}$  Generation

of the first projection axis was, the smaller the numbers of violations in terms of "Established prohibited working patterns", "Fairness of the number of working times on night or midnight shifts among nurses" and/or "The prescript number of working times per month on night or midnight shifts in each nurse" were. On the other hand, the coefficients of  $Obj_1$ ,  $Obj_2$  on the second projection axis shows positive values and that of  $Obj_5$  shows negative value. It means that the bigger the value of the second projection axis was, the bigger the number of violations in terms of "Level of requisite nurses in each shift per day" and/or "The number of requisite nurses in each team per day" and the smaller that of "Fairness of the number of working times on night or midnight shifts among nurses" were.

# B. Investigation of visualization result

Figure 2 shows the visualization result of the acquired Pareto solutions at the  $100,000^{th}$  generation. The visualized Pareto solutions had the linearity between the first and second projection axes. In Table 1, the positive and negative of coefficients of  $Obj_2, Obj_3$  and  $Obj_5$  between the first and second projection axes were corresponding each other. In addition, though the positive and negative of  $Obj_7$  was not corresponding, the eigen value of the first projection axis was predominantly bigger than the second one and coefficient of  $Obj_7$  on the first projection axis was big negative value. In consideration of them, the upper right Pareto solutions or those belonging to cluster 2, 5 represented scheduling tables (nondominated solutions) with smaller number of violations in terms of  $Obj_3$ ,  $Obj_5$ ,  $Obj_7$  and bigger that of  $Obj_2$ , and the left lower solutions and cluster 4 had inverse characteristics. Cluster 1 or 3 were the middle of them or well-balanced in terms of the number of violations. These

TABLE I

	Eigen Vector											
Projection Axis No.	Eigen Value	$Obj_1$	$Obj_2$	$Obj_3$	$Obj_4$	$Obj_5$	$Obj_6$	$Obj_7$				
1	2.038	-0.39	0.30	-0.44	-0.09	-0.44	-0.17	-0.57				
2	0.298	0.58	0.43	-0.17	0.01	-0.58	-0.23	0.24				
3	0.189	-0.56	-0.46	0.002	0.55	-0.14	-0.28	-0.26				
4	0.055	0.18	0.36	-0.01	-0.69	0.45	-0.23	0.31				
5	0.0034	-0.15	-0.35	0.01	0.70	-0.47	0.22	-0.31				
6	0.0004	-0.15	-0.35	0.01	0.70	-0.47	0.22	-0.31				
7	0.0001	0.15	0.35	-0.01	-0.70	0.47	-0.22	0.31				

EIGEN VALUES AND EIGEN VECTORS BY FMDA

investigations clarified that there was trade-off relationship between the objective function  $Obj_3$ ,  $Obj_5$ ,  $Obj_7$  and  $Obj_2$ in Pareto solutions at the  $100,000^{th}$  generation.

# C. Characteristics of clusters

The proposed method can also compare the cluster centers and investigate the characteristics of clusters. Table 2 shows the fitness values (the number of violations) of objective functions on the cluster centers. This table shows actual fitness values of the clusters were corresponding to the characteristics of them described in the previous section. Figure 3 shows an example of the acquired scheduling table belonging to cluster 5. In this way, the proposed method enables us to support decision-making for users such as selection of the satisfied solutions efficiently.

In addition, the proposed method can generate the visible space which separates the acquired clusters as far as possible by FMDA. In Fig. 2, only the cluster 4 was separated from other clusters in visible space, however the other clusters overlapped each other and they were not completely separated. The clusters except for the cluster 4 overlapped equally in multi-dimensional objective function space, which means that the continuous Pareto solutions could be acquired around these clusters. Acquisition of continuous Pareto solutions is one of the most important indexes to evaluate performance of the optimization method in multi-objective optimization problems. It is supposed that the Pareto solutions in the area of these clusters were continuous and variety. On the other hand, in the area of cluster 4, bigger number of violations of  $Obj_3$ ,  $Obj_5$ ,  $Obj_7$  and smaller that of  $Obj_2$ , were less density among individuals and discontinuous, which means that the evolution in this area was not enough and there were some unsearched areas.

### D. Visualization of search process

Figure 4 shows the visualization result of the acquired Pareto solutions at the  $110,000^{th}$  generation. This figure uses the same projection axes at the  $100,000^{th}$  generation. We can easily compare Fig. 4 with Fig. 2 and grasp the improvement of the evolution in terms of the acquired Pareto solutions



Fitness Value ( $Obj_{p}, Obj_{2}, Obj_{3}, Obj_{6}, Obj_{5}, Obj_{6}, Obj_{7}$ ) =(4,50,11,5,8,72,41)

Fig. 3. Example of Acquired Scheduling Table

in these 10,000 generations. It is confirmed in fig.4 that a lot of new nondominated solutions were generated around cluster 4 where they had not searched well at the  $100,000^{th}$  generation. One of the characteristics of NSGA-II, which is that the particular chromosomes with less density in the Pareto population are given the priority to be applied genetic operations, worked well there after  $100,000^{th}$  generation. It shows the possibility that the proposed method enables us not only to visualize the acquired Pareto solutions but also to grasp the search process.

## V. CONCLUSIONS

This paper proposed the visualization method using FCM and FMDA for Pareto solutions having multi-objective fitness values as one of the approach of mining of solutions. This paper applied the proposed method to the Pareto solutions of NSP acquired by NSGA-II and investigated the effectiveness of this method. The proposed enabled us to interpret or analize the acquired Pareto solutions such as the distributed structures of Pareto solutions in multi-dimensional space, the relationships among the objective functions and the characteristics of the clusters through the meaning of projection axes. This paper also showed that the proposed method has

TABLE II

 $\overline{Obj}_3$  $\overline{Obj}_5$  $\overline{Obj}_7$  $\overline{Obj_2}$  $\overline{Obj}_4$  $Obj_6$ Cluster No.  $Obj_1$ Cluster1 1.45 33.8 56.7 4.32 17.2 45.8 136.0 Cluster2 2.24 104.9 40.5 25.6 2.95 10.6 41.0 Cluster3 1.76 29.7 103.1 4.50 17.3 49.1 144.3 Cluster4 3.41 29.1 183.9 0.75 20.1 45.2 241.5 2.27 73.3 Cluster5 43.5 10.1 4.53 8.8 44.5 Average of all Pareto solutions 2.03 38.1 47.4 3.81 13.0 44.9 114.0





Fig. 4. Visualization Result at the  $110,000^{th}$  Generation

the possibility to grasp the search process visually.

Future work is more investigation of the proposed method comparing with nonlinear method like SOM and other linear methods. We will apply the method to the improvement of search performance by grasping the features of the search process in different genetic operators. We will also try to develop another effective approach of mining of solutions.

## VI. ACKNOWLEDGMENTS

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