Diversity Maintenance Mechanism for Multi-Objective Genetic Algorithms using Clustering and Network Inversion

Tomoyuki Hiroyasu[1], Kenji Kobayashi[2], Masashi Nishioka[2], Mitsunori Miki[3]

[1] Faculty of Life and Medical Sciences, Doshisha University, 1-3 Tatara Miyakodani Kyotanabe, Kyoto, Japan,
[2] Graduate School of Engineering, Doshisha University
[3] Faculty of Science and Engineering, Doshisha University
(tomo@is,kkobayashi@mikilab,mnishioka@mikilab,mmiki@mail).doshisha.ac.jp

Abstract. One of the major issues in applying multi-objective genetic algorithms to real-world problems is how to reduce the large number of evaluations. The simplest approach is a search with a small population size. However, the diversity of solutions is often lost with such a search. To overcome this difficulty, this paper proposes a diversity maintenance mechanism using clustering and Network Inversion that is capable of preserving diversity by relocating solutions. In addition, the proposed mechanism adopts clustering of training data sets to improve the accuracy of relocation. The results of numerical experiments on test functions and diesel engine emission and fuel economy problems showed that the proposed mechanism provided solutions with high diversity even when the search was performed with a small number of solutions.

1 Introduction

Multi-objective genetic algorithms (MOGAs) are strong optimization methods that can derive a Pareto-optimal set in a single run [1, 2]. However, in real-world problems, such as large-scale design problems [3, 4], the reduction of evaluation calls becomes an essential issue due to their high computational cost. Two major approaches have been proposed for this issue: the response surface method [5–7] and search using small population size [8] (SSP strategy). In this paper, an effective SSP mechanism is discussed. SSP is a simple approach for reducing the calculation cost. However, solution diversity in the objective space tends to be lost. We have proposed a diversity maintenance mechanism using an Artificial Neural Network (ANN) [9] to preserve high diversity, which relocates the converged solutions to solutions with a uniform distribution. In this relocation, it is necessary to perform inverse analysis that estimates the design values from the fixed objective values, because the relocation must be conducted in the objective space. In our previous paper, inverse function by ANN was adopted, but it showed poor performance in high-dimensional or multi-modal problems. In this paper, new diversity maintenance mechanism based on Network Inversion [10, 11] and clustering of ANN training data is proposed to solve these difficulties.

2 Mode of Inverse Analysis and Necessity of Clustering

2.1 Mode of Inverse Analysis in the Proposed Mechanism

In the proposed mechanism, Network Inversion (NI) [10, 11] is applied for inverse analysis, which is a technique using an approximation function with the same structure as the objective function. This mode is advantageous with regard to high-dimensional problems. In the conventional mode based on inverse function, it is difficult to relocate solutions appropriately, because many outputs should be estimated from few inputs in high dimensions. On the other hand, NI preserves the input/output relationship of the objective function, and is effective in high dimensions. Most studies concerned with ANN focus only on an approximation of the objective function and local search [12, 13]. On the other hand, ANN was used in this study to relocate the solutions and restore the solution diversity.

2.2 Necessity of Clustering

The filtration of training data set to improve the approximation accuracy of NI is also discussed. To create a good approximation function with few data, the following two conditions should be satisfied:
(i). Training data set exists in a narrow area.
(ii). Approximation function is a monotone in approximation area.

A case where a function pole exists in a training area is illustrated in Fig.1 to discuss the importance of these conditions.

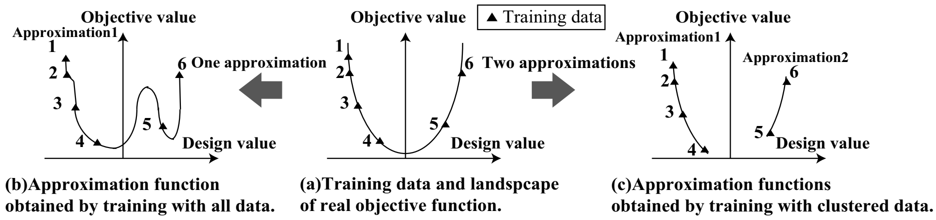

Fig. 1. Case where a function pole exists in a training area and its handling

In Fig.1, Fig.1(c) which satisfies both (i) and (ii) by dividing the training data set into two groups, is a good method of training when a function pole exists in the training area. Whether there is a function pole in the training area can be judged according to the neighbor relationship of the data. To check this, it is necessary to make two sorting lists of all data, which are sorted by design values and objective values in ascending order. When two adjacent data points of an arbitrary data set are the same in both lists, the training data set is defined as having the same neighbor relationship. For example, when all training data in Fig.1(a) are sorted by design and objective values (Fig.1(b)), each list becomes (1,2,3,4,5,6) and (4,5,3,2,6,1). In this case, the data set has a different neighbor relationship. On the other hand, in Fig.1(c), training data are divided into two groups: (1,2,3,4,) and (5,6). If the same sorting procedure is performed on both groups, the neighbor relationship becomes the same. In this paper, we propose a clustering method that can divide training data sets into groups with the same neighbor relationship.

3 Diversity Maintenance Mechanism by Clustering and Network Inversion

The proposed mechanism is composed of MOGA search, clustering, training ANNs, and relocation, and the latter 3 processes are used to restore diversity. The concept of the proposed mechanism is illustrated in Fig.2.

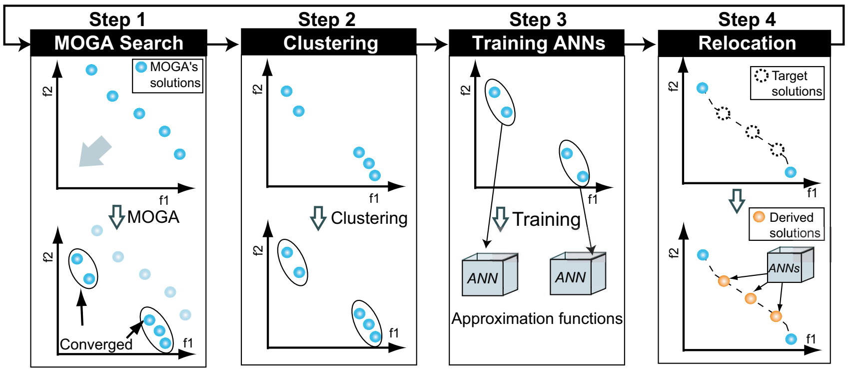

Fig. 2. Concept of proposed mechanism

The first application of the restoration process is when all archive solutions become the non-dominated solutions (NDS), and is applied uniformly in the remaining search. The algorithm is described below:

Step 1:MOGA search: MOGA search is performed until application condition of the diversity restoration is met. After application of the diversity restoration, MOGA search is conducted for specified number of generations.
Step 2:Clustering: Clustering is applied to the NDS obtained by MOGA.
Step 3:Training ANNs: ANNs are trained based on a set of clustered solutions obtained in Step 2.
Step 4-1:Linear interpolation: A linear line passing through a set of n NDS is obtained by interpolation.
Step 4-2:Locating target solutions (TS): All solutions are removed except those at the edges, and $n-2$ TS are located uniformly on the interpolated line.
Step 4-3:Inverse analysis: Inverse analysis is performed with NI, and design values corresponding to each objective value of TS are derived.
Step 4-4:Relocation: Obtained design values are evaluated using the real objective function. Then, archive and solutions obtained by NI are combined, and the archive update mechanism of MOGA is executed. Return to Step 1 if the terminal condition is not satisfied.

3.1 Clustering (Step 2)

A clustering algorithm is proposed to obtain a set of solutions with the same neighbor relationship. It judges the neighbor relationship by calculating the Euclidean distance between one solution and the others. The solution used to calculate the distance is defined as the base solution, and the solutions with minimum or maximum value in any objective function are defined as edge solutions. Furthermore, this operation is applied only to n NDS of archive, because it showed superior results in the preliminary experiment. The clustering procedure is described below, and the clustering of the solutions in Fig.3 is shown in Fig.4

Step 2-1: ID is assigned to k NDS in ascending order regarding f1 ($i = 0$).
Step 2-2: A base solution is fixed ($i = 0$: solution with ID=1, $i = 1$: ID=k).
Step 2-3: Euclidean distances between the base solution and the others are calculated in the design space, and a sorted list of IDs is made by the distance in ascending order.
Step 2-4: Consecutive solutions from the head of the sorted list with its IDs in ascending ($i = 0$) or descending ($i = 1$) order are selected as setA_i
Step 2-5: If $i = 0$, return to Step 2-2 and update the base solution ($i = 1$).
Step 2-6: When setA_0=setA_1, a cluster is created from the solutions of set A_0, and the process is terminated. When either set becomes the subset of the other, the solutions of the subset are adopted as a cluster, and the process is terminated. Otherwise, only sets with the edge solution included are selected as the new NDS set, and the clustering process is repeated to it.

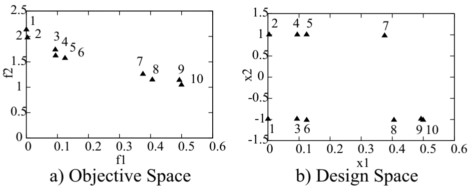

Fig. 3. Distribution of a data set

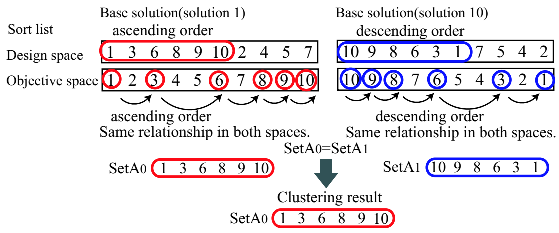

Fig. 4. Concept of clustering

This algorithm does not require the number of clusters to be assigned beforehand, because only clusters that include the edge solution are obtained.

3.2 Training ANNs (Step 3)

In Step 3, training ANNs is performed regarding design values as input and objective values as output by Backpropagation (BP). Solutions from clustering in Step 2 are adopted as a training data set. With BP, output error is minimized based on the gradient method by considering the weights of the network as the source of error and adjusting it.

3.3 Linear Interpolation and Location of Target Solutions (Steps 4-1 and 4-2)

In this section, we describe how the objective values of TS are determined. First, a linear interpolation line is obtained (Step 4-1). For this interpolation, a linear interpolation method is adopted, because it showed more positive results in preliminary experiments than two-dimensional interpolation. Next, TS are located on the interpolated line such that the distances on the interpolated line between the neighboring solutions become the same. As it is difficult to set TS in many objectives (more than three), this paper focuses on two-objective problems. The scheme of locating TS is shown in Fig.5.

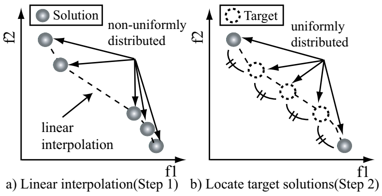

Fig. 5. Concept of locating TS

3.4 Inverse Analysis (Step 4-3)

In this step, input values are estimated from fixed output values using ANNs trained in Step 3. The principle of inverse estimation by NI is the same as that of BP. However, the source of error is considered to be the input values, and they are adjusted instead of the weights of the network. From the process described above, design values x of TS are estimated. In addition, training cost of ANNs and calculation cost of NI are relatively small in comparison with the evaluation cost of GA, and these costs are not discussed in this paper.

3.5 Relocation (Step 4-4)

Estimated design values from Step 4-3 are evaluated by the objective function, and real-objective values are obtained. Next, the archive update mechanism is applied to a set of solutions composed of solutions of inverse analysis and MOGAs. With this, a superior set of solutions with high accuracy and diversity can be selected. In addition, even if TS cannot be obtained properly, the search performance will not be degraded because the updating mechanism eliminates them and the solutions before relocation are adopted.

4 Numerical Experiments Through Test Functions

The effectiveness of the proposed mechanism was verified through numerical experiments. Search performance was compared by Angular Cover Rate (ACR) for diversity and GD for accuracy [14]. In ACR, domains in which solutions exist are divided uniformly into the number of search population size by the angle, and it counts how many domains are covered by derived solutions. On the other hand, GD measures the accuracy by calculating the distance between derived solutions and Pareto-optimal solutions. In all experiments discussed in this section, NSGA-II is employed for MOGAs of the proposed mechanism, and population size is set to 10 [8], because the search with a small number of solutions is assumed. In addition, crossover rate is 1.0, and mutation rate is 1.0/gene length. The concept of ACR and GD is illustrated in Fig.6 and Fig.7.

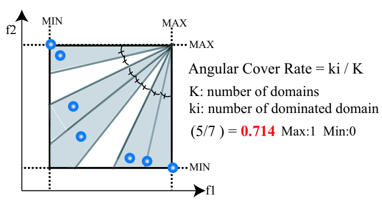

Fig. 6. Concept of ACR

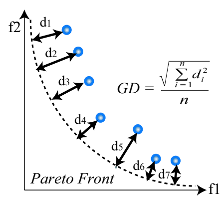

Fig. 7. Concept of GD

In this section, the following three experiments are discussed.

1. Effectiveness of clustering.
2. Improvement of diversity by the proposed mechanism.
3. Diversity maintenance and accuracy by iterating the proposed mechanism.

4.1 Accuracy of an Approximation by Clustering and NI

The differences in performance between NI and NI with clustering were verified using multi-modal function ZDT4 [15] with 2-dimensions. The training data set and the results are shown in Fig.8 and Fig.9, respectively.

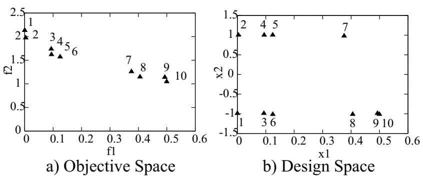

Fig. 8. Test data set

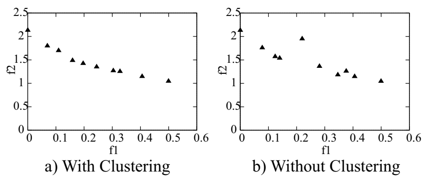

Fig. 9. Effectiveness of NI with clustering

The results shown in Fig.9 indicate that when the neighbor relationships in both spaces are different, clustering may provide more accurate approximation.

4.2 Effect of the Proposed Mechanism for Diversity

In this experiment, MOGA search and the proposed mechanism were compared to examine the effects of the proposed mechanism on diversity. Test functions were ZDT1, ZDT2, and ZDT4 with three patterns of dimensions (2,5,10), and the number of generations for GA was 100. The results are shown in Fig.10.

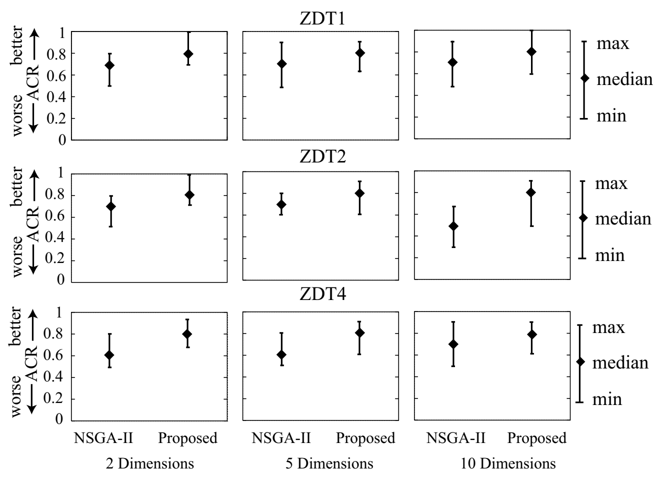

Fig. 10. ACR (Max, Median, Min) in ZDT1, ZDT2, ZDT4

Fig.10 shows the minimum, median, and maximum of ACR at 30 runs. From these results, we can infer that the proposed mechanism provides solutions with high diversity even in high dimensions.

4.3 Effect of the Iteration of the Proposed Mechanism

The effects of diversity maintenance by the proposed mechanism were verified. In ZDT1 and ZDT2, generation was set to 100, and the number of applications of the proposed mechanism was set to 5. In ZDT4, each parameter was set to 300 and 15, respectively. In addition, the number of dimensions was 10. In this experiment, the effects of diversity maintenance by the proposed mechanism were validated by the transition of ACR. The results are shown in Fig.11.

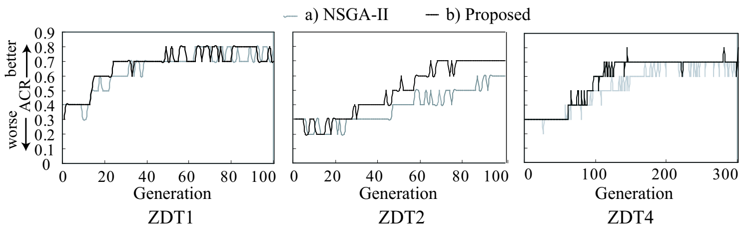

Fig. 11. Transition of ACR in ZDT1,ZDT2,ZDT4

Fig.11 indicates the median of ACR measured by the generation. These results show that the search with the proposed mechanism can maintain high diversity compared to only using MOGAs. Next, the influence regarding the accuracy by the proposed mechanism was verified by GD. The results on median and standard deviation are shown in Table.1. The number of evaluations was the same in both methods.

Table 1. Comparison of GD

		ZDT1	ZDT2	ZDT4
NSGA-II	Median	0.209	0.348	3.53
	Standard deviation	0.106	0.128	1.66
Proposed	Median	0.238	0.362	3.06
	Standard deviation	0.130	0.214	1.31

As shown in Table.1, both methods showed comparable accuracy. From these results, we concluded that the proposed mechanism can maintain solution diversity without deterioration of solution accuracy even in high dimensions.

5 Numerical Experiments Through Real-World Problem

The effectiveness of the proposed mechanism was verified by application to the diesel engine emission scheduling problem.

5.1 Diesel engine Fuel Emission Scheduling Problem

Diesel engines have considerable advantages with regard to durability, fuel economy, and reduced CO_2 emission. However, in recent years, emission regulations for automobile engines have become stricter because of the adverse influence on the environment. Therefore, there is a great deal of research interest in reducing emissions to meet the regulations [16].

A diesel engine works by compressing air in a cylinder and injecting a liquid fuel. However, it also emits large amounts of both nitric oxide (NO_x) and particulate matter (PM), including soot. The amounts of these emissions are determined by the scheduling of fuel emission. Therefore, the emission characteristics were optimized from the perspective of engine combustion to achieve low emission. This optimization problem is called the diesel engine emission scheduling problem, and minimizes the following objectives:

– The amount of NO_x
– The amount of soot
– The amount of specific fuel consumption (SFC)

This problem should be optimized simultaneously due to the trade-off relationships between NO_x and soot or SFC. These objective values are calculated by simulation with the phenomenological model HIDECS [17, 18]. Design variables are Start Angle, Exhaust Gas Recirculation Rate (EGR Rate), Swirl Ratio, Boost Pressure, and the shape of injection [19].

In this section, it is examined whether the proposed mechanism can improve the diversity, and also if the diversity can be preserved by iterating them.

5.2 Effects of Relocation in the Diesel Problem

The effects on diversity were verified when the proposed mechanism was applied once. In all of the following problems, only SFC and NO_x were focused upon because the mechanism can only be utilized with two-objective problems. Population size was set to 10 and the number of generations was 50. The other GA parameters were the same as in section 4. The results are shown in Fig.12.

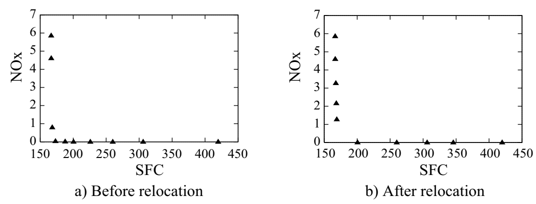

Fig. 12. Effect of the relocation of the proposed mechanism

As shown in Fig.12, the diversity can be improved by the proposed mechanism in the diesel engine problem.

5.3 Effects of Iteration in the Diesel Problem

The effects on diversity maintenance of the proposed mechanism were verified. In this experiment, the transition of ACR was examined during a search. The plot graphs of obtained NDS at 30 runs were compared to measure the accuracy, because Pareto-optimal solutions in this problem were not known and GD could not be employed as an indicator. The number of generations was set to 50 and the number of applications of the proposed mechanism was set to 10. The number of evaluations was the same in both methods. The first experimental results of the transition of ACR are illustrated in Fig.13. Fig.13 shows that the proposed mechanism can provide solutions with higher diversity during a search than the conventional search.

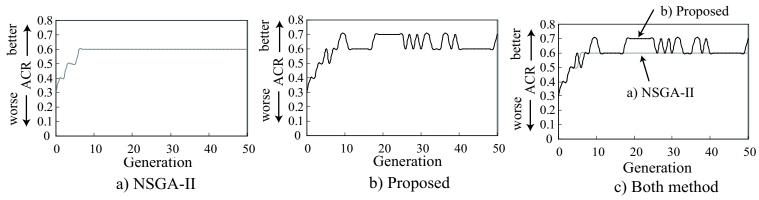

Fig. 13. Transition of ACR in diesel problem

In the second experiment, the influence of iteration on the search performance was examined by plotting all obtained NDS at 30 runs in Fig.14.

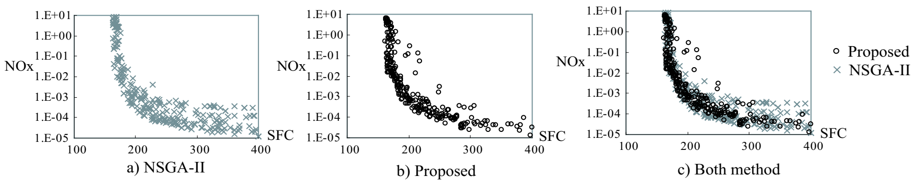

Fig. 14. All NDS obtained by both methods in diesel problem

Fig.14 indicates that the search performance of the proposed mechanism is comparable to the conventional method with regard to accuracy. From these results, we concluded that the proposed mechanism can provide solutions with high diversity without deterioration of the search performance in the diesel engine emission scheduling problem.

6 Conclusions and Future Work

In this paper, a new diversity maintenance mechanism was proposed that hybridizes MOGAs with a small population size and the process of restoring diversity by NI. This mechanism involves MOGA search, clustering, training ANNs, and relocation, and diversity can be preserved by iteration.

The effectiveness of the proposed mechanism was examined through application to benchmark problems and the diesel engine emission scheduling problem. The results showed that the proposed mechanism can provide solutions with high diversity even in high dimensions and the search with 10 solutions. In future studies, we will examine the appropriate number of solutions for the search, and how to apply the proposed mechanism to many-objective problems (more than 3).

References

1. K.Deb, S.Agrawal, A.Pratab, and T.Meyarivan. A Fast Elitist Non-Dominated Sorting Genetic Algorithm for Multi-Objective Optimization: NSGA-II. In *KanGAL report 200001, Indian Institute of Technology, Kanpur, India*, 2000.
2. E.Zitzler, M.Laumanns, and L.Thiele. SPEA2: Improving the Performance of the Strength Pareto Evolutionary Algorithm. In *Technical Report 103, Computer Engineering and Communication Networks Lab (TIK), Swiss Federal Institute of Technology (ETH) Zurich*, 2001.

3. K.Chiba, S.Obayashi. High-Fidelity Multidisciplinary Design Optimization of Aerostructural Wing Shape for Regional Jet. In *23rd Applied Aerodynamics Conference*, 2005.
4. T.Hiroyasu, M.Miki, J.Kamiura, S.Watanabe, and H.Hiroyasu. Multi-Objective Optimization of Diesel Engine Emissions and Fuel Economy using Genetic Algorithms and Phenomenological Model. In *SAE 2002 Powertrain and Fluid Systems Conference*.
5. T.Shirai, M.Arakawa, and H.Nakayama. Approximate Multi-Objective Optimization Using RBF Network. In *The Computational Mechanics Conference, Vol18th*, pp. 759–760, 2005.
6. Julio L. Peixoto. Hierarchical Variable Selection in Polynomial Regression Models. *The American Statistician*, Vol. 41, No. 4, pp. 311–313, 1987.
7. J. Sacks et al. Design and Analysis of Computer Experiments 4. *Statistical Science*, Vol. 4, pp. 409–435, 1989.
8. S.Obayashi, D.Sasaki, and A.Oyama. Finding Tradeoffs by Using Multiobjective Optimization Algorithms. In *Transactions of JSASS Vol47, No.155*, pp. 51–58, 2004.
9. K.Kobayashi, T.Hiroyasu, and M.Miki. Mechanism of Multi-Objective Genetic Algorithm for Maintaining the Solution Diversity Using Neural Network. In *Lecture Notes in Computer Science*, Vol. 4403, pp. 216–226. Springer, 2007.
10. A.Linden and J.Kindermann. Inversion of multilayer nets. In *Proc.Int.Joint conf.on Neural Networks*, pp. 425–430, 1989.
11. T.Ogawa and H.Kaneda. Complex-Valued Network Inversion for Solving Complex-Valued Inverse Problems. In *Bulletin of science and engineering, Takushoku University, Vol.9, No.4*, pp. 83–84, 2006.
12. A.G.Cunha and A.Vieira. A Hybrid Multi-Objective Evolutionary Algorithm Using an Inverse Neural Network. In *Hybrid Metaheuristics*, pp. 25–30, 2004.
13. S.F.Adra, I.Hamody, I.Griffin, and P.J.Fleming. A Hybrid Multi-Objective Evolutionary Algorithm Using an Inverse Neural Network for Aircraft Control System Design. *2005 IEEE Congress on Evolutionary Computation (CEC'2005)*, Vol. 1, pp. 1–8, 2005.
14. K.Deb. Multi-Objective Optimization using Evolutionary Algorithms. pp. 326-327. John Wiley and Sons, Chichester, England.
15. K.Deb and T.Meyarivan. Constrained Test Problems for Multi-Objective Evolutionary Optimization. In *KanGAL report 200005, Indian Institute of Technology, Kanpur, India*, 2000.
16. Y.Aoyagi. A Survey of Existing Emission Reduction Technology for Gasoline-powered Engine and Future Prospect. Vol. 55, No. 9, pp. 10–16, September 2001.
17. H.Hiroyasu, T.Kadota, and M.Arai. Development and Use of a Spray Combustion Modeling to Predict Diesel Engine Efficiency and Pollutant Emissions (Part 1 Combustion Modeling). *Bulletin of the JSME*, Vol. 26, No. 214, pp. 569–575, April 1983.
18. H.Hiroyasu, T.Kadota, and M.Arai. Development and Use of a Spray Combustion Modeling to Predict Diesel Engine Efficiency and Pollutant Emissions (Part 2 Computational Procedure and Parametric Study). *Bulletin of the JSME*, Vol. 26, No. 214, pp. 576–583, April 1983.
19. S.Itoh and K.Nakamura. Reduction of Diesel Exhaust Gas Emission with Common Rail System. Vol. 55, No. 9, pp. 46–52, September 2001.