

Partial Sampling Operator and Tree-structural Distance for Multi-objective Genetic Programming

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Abstract: This paper describes a technique on an optimization of tree-structure data, or genetic programming (GP), by means of a multi-objective optimization technique. NSGA-II is applied as a frame work of the multi-objective optimization. GP wrecks bloat of the tree structure as one of the major problem. The cause of bloat is that the tree structure obtained by the crossover operator grows bigger and bigger but its evaluation does not improve. To avoid the risk of bloat, a partial sampling (PS) operator is proposed instead to the crossover operator. Repeating processes of proliferation and metastasis in PS operator, new tree structure is generated as a new individual. Moreover, the size of the tree and a tree-structural distance (TSD) are additionally introduced into the measure of the tree-structure data as the objective functions. And then, the optimization problem of the tree-structure data is defined as a three-objective optimization problem. TSD is also applied to the selection of parent individuals instead to the crowding distance of the conventional NSGA-II. The effectiveness of the proposed techniques is verified by applying to the double spiral problem.

1 INTRODUCTION

A technique of genetic programming (GP)(Koza, 1992; Koza, 1994) is an algorithm to optimize structured data based on a genetic algorithm(Goldberg, 1989; Mitchell et al., 1996). GP is applied to various fields such as program synthesis(David and Kroening, 2017), function generations(Jamali et al., 2017) and rule set discoveries(Ohmoto et al., 2013). Although GP is very effective for optimizing structured data, it has several problems such as getting into a bloat, inadequate optimization of constant nodes, being easily captured in local optimal solution area when applied to complicated problems. The main cause of bloat is a crossover operator which exchanges partial trees of parent individuals(Nordin et al., 1995; Angeline, 1997; Angeline, 1998; De Jong et al., 2001), where this paper focuses on the optimization of tree-structure data by means of GP. Several techniques to reduce the bloat have been proposed by improving the simple crossover operation(Koza, 1994; De Bonet et al., 1997; Mühlenbein and Paass, 1996; Ito et al., 1998; Langdon, 1999; Francone et al., 1999). Although these methods have successfully inhibited bloat to a certain extent, effective search has not necessarily been performed. Moreover, there is no theoretical basis that crossover is effective for optimizing the tree-structure data.

Apart from reduction of the bloat, a search method for optimizing the graph structure has been proposed(Karger, 1995). Although this method is suitable for searching various structural data consisting of nodes and branches, the algorithm is complicated and the computation cost is high.

In this paper, we exclude the crossover operator which is the cause of bloat in GP, and propose a partial sampling (PS) operator as a new operator for GP instead. In PS operator, first of all, a partial sample of a partial tree structure is extracted from several individuals of a parent individual group by a proliferation. Next, the partial tree structure obtained by the proliferation is combined with a new tree structure by a metastasis. In this paper, two types of metastasis are prepared for GP, one that depends on the original upper node and the other that does not. Repeating the proliferation and the metastasis regenerates a new tree-structure data for the next generation.

In addition, in this paper, MOEA technique for suppressing bloat and acquire many kinds of various tree-structure data is applied for GP by adding the size and the distance of the tree-structure data to the evaluation. One of the newly added objective functions is the size of the tree-structure data. Furthermore, the relative position of the target individual in the population in terms of the tree-structural distance (TSD) is also evaluated as an objective function. The tree-

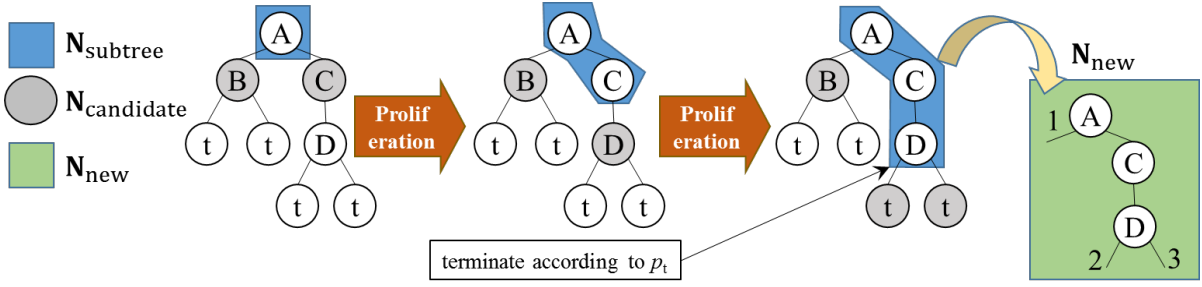


Figure 1: The initial proliferation in PS operator.

structure data optimization problem is formulated as a three objective optimization problem by defining these three objective functions.

NSGA-II(Deb et al., 2000; Deb, 2001) is applied to this three objective optimization problem. In the conventional NSGA-II, a crowding distance (CD) is applied for ranking the front set overflowing from the parent group. In optimizing the tree-structure data, we can not maintain diversity of the population by focusing only on the value of the objective function and storing the solution near the extreme solution. In this paper, TSD is applied, instead of CD, for ranking the front set overflowing from the parent group.

In order to verify the effectiveness, the proposed technique and the conventional techniques is applied to a double spiral problem (De Bonet et al., 1997; Yang and Kao, 2000). The double spiral problem is a classification problem containing two classes of point sets arranged on a spiral shape to be classified with a function. This problem is well known as one of difficult problem to solve with a neural network. In this paper, GP obtains the classifying function composed of the finite mathematical elements.

2 PARTIAL SAMPLING OPERATOR FOR MATING

One of the main causes of bloat is the crossover operator generally applied in the conventional GPs, used for regenerating a new tree-structure data. This paper proposes to exclude the crossover operator from the conventional GP and to apply PS operator for regeneration of a new tree-structure data instead of the crossover operator. The PS operator creates a new tree-structure data by partially sampling tree structures from a parent individual and joining them together. This procedure is called a proliferation. The proliferation is terminated according to the probability, p_t . Partially sampled subtree structures by the proliferation are combined together by a metastasis. Two types of the metastasis are prepared, one that de-

pends on the original upper node and the other that does not. We call the the former as an upper node depend metastasis and the latter as a random metastasis.

In the initial proliferation, a root node, $n_{i,root}$, of an individual, $indiv_i$, randomly selected from a parent group \mathbf{P}^s is copied to a set $\mathbf{N}_{subtree}$ as shown in Fig.1. The initial proliferation is started from the root node, $n_{i,root}$, of the individual, $indiv_i$. In this example, the starting root node contains an identification, A. Let $\mathbf{N}_{candidate}$ be a set of all lower nodes under the node of $\mathbf{N}_{subtree}$, where that node is not selected as a node of $\mathbf{N}_{subtree}$ yet. One node is randomly selected from $\mathbf{N}_{candidate}$ and copied to $\mathbf{N}_{subtree}$. The proliferation terminates according to the proliferation terminate probability, p_t , or when $\mathbf{N}_{candidate} = \emptyset$. When the proliferation is terminated, the set $\mathbf{N}_{subtree}$ thus obtained is copied to \mathbf{N}_{new} , where is a set of nodes as a new tree-structure data. The set $\mathbf{N}_{subtree}$ is initialized to \emptyset . Furthermore, the root node of the partial tree structure \mathbf{N}_{new} in the initial proliferation is randomly generated in a low probability on the initial proliferation.

In the conventional GP with variable structure length, small partial structures are assembled by an regenerating operator, for example, crossover or mutation, and these partial structures are combined to generate a new tree-structure data of a large size(Poli and Langdon, 1998; Poli et al., 2008). When the conventional GP increases the average size of the tree-structure data, the size of the partial structure also preserved for the next generation increases. Therefore, the probability, p_t is scheduled as follows.

$$p_t^0 = \frac{1}{\text{AverageSize}(\mathbf{R}^g)}, \quad (1)$$

$$p_t^{g+1} = (p_t^g - p_t^0) \frac{\frac{1}{\text{Succeed}(\mathbf{P}^g)} - p_t^0}{\frac{1}{\text{Succeed}(\mathbf{R}^g)} - p_t^0} + p_t^0, \quad (2)$$

where p_t^0 denotes the probability, p_t , at the initial generation, p_t^g denotes the probability, p_t , at the g -th generation, \mathbf{R}^g denotes a population at the g -th generation, $\mathbf{P}^g \subset \mathbf{R}^g$ denotes the parent group at the g -th

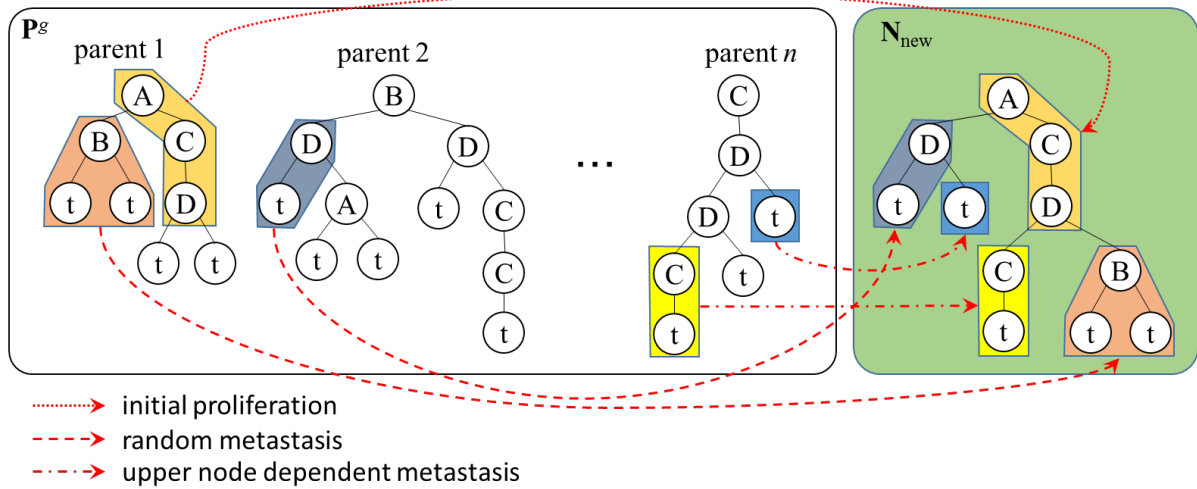


Figure 2: Outline of how a new tree structure is created by PS operator.

generation, $AverageSize(\cdot)$ denotes a function returning the average size of the tree set, and $Succeed(\cdot)$ denotes a function returning the average size of the partial tree structure that the argument set takes over from the previous generation. Scheduling the probability, p_t , as shown above prevents the size of the partial tree structure from explodingly increasing.

A partial tree structure is grown by applying one of two kinds of metastasis to the partial tree structure obtained by the initial proliferation. One of two kinds of metastasis is a random metastasis. The random metastasis activates according to a metastasis selection probability, p_{met} . The other one metastasizes depending on the upper node. The upper node dependent metastasis activates according to the probability, $1 - p_{met}$. The partial tree structure N_{new} shown in the Fig.1 has three empty branched numbered as 1, 2 and 3. The branch 1 has the upper node A, and the branches 2 and 3 have upper node D. Now, suppose that the branch 1 is selected as a target of the upper node depend metastasis. In the next proliferation, a node having the upper node A is selected from the parent group, P^g . On the other hand, if the random metastasis is applied to the partial tree structure N_{new} , the beginning node for the next proliferation is randomly selected from the parent group, P^g .

A new node is selected from the parent group, P^g , according to the decided metastasis type. This node is not necessarily a root node. The proliferation is started from the selected node again.

By repeating the proliferation and the metastasis, new tree-structure data is generated as shown in Fig.2. However, when the metastasis applied to only one parent individual, or when a parent individual having the same structure as the generated tree structure, the

generated tree structure is eliminated and PS operator is performed again. The terminal nodes are given as a random number in a low probability, where this is based on the conventional mutation idea.

3 MULTI-OBJECTIVE GENETIC PROGRAMMING

Optimizing the tree-structure data based only on the index of its own goodness brings problems that causes bloat but also that the optimization is caught in a local optimum region. Depending on the structure of the local optimum region, the optimization stagnates, causing an illusion as if it were the ultimate optimal solution. To avoid the risk of such the problems, this paper, therefore, proposes a technique to optimize based on the size of the tree structure and TSD in the population in addition to the index of the goodness of tree structure.

In this paper, three objective functions are defined as follows to be used for the multi-objective optimization. An objective function according to the goodness of an individual, $indiv_i$, is described by the following equation.

$$h_1(indiv_i) = performance(root_i), \quad (3)$$

where $root_i$ denotes a root node of the individual, $indiv_i$, and $performance(root_i)$ denotes a function that returns value of the goodness of the tree structure beginning from the root node, $root_i$.

An objective function according to the size of tree structure is defined by the following equation.

$$h_2(indiv_i) = \frac{1}{Size(root_i)}, \quad (4)$$

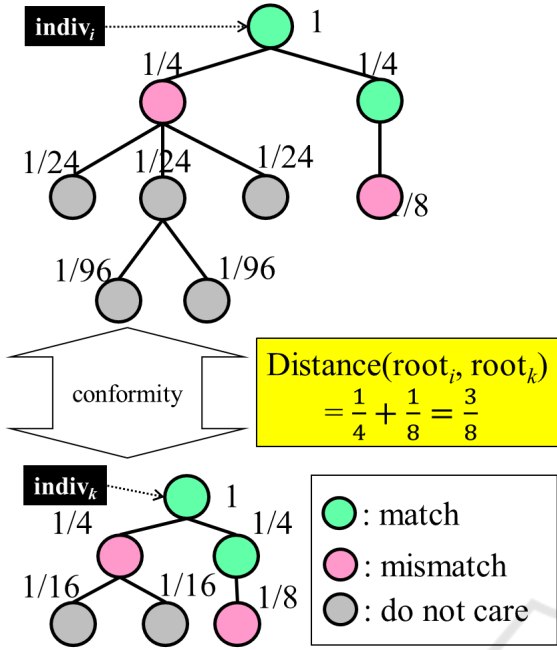


Figure 3: An example of giving weights to the tree structure and TSD.

where $\text{Size}(\text{root}_i)$ denotes a function that returns the number of the nodes of the tree structure beginning from the root node, root_i .

An objective function according to average of TSD in the population is defined by the following equation.

$$h_3(\text{indiv}_i) = \frac{1}{N_{\text{pop}}} \sum_{k=1}^{N_{\text{pop}}} \text{Distance}(\text{root}_i, \text{root}_k), \quad (5)$$

where N_{pop} denotes the size of the population, and $\text{Distance}(\text{root}_i, \text{root}_k)$ denotes a function that returns TSD between indiv_i and indiv_k . In order to calculate TSD, weights are given to all the nodes of the tree structured data by means of the following steps, when the tree structured data is initially generated. An example of giving weights to the tree structure is shown in Fig.3.

- (Step 1)** Give weight 1 to the root node.
- (Step 2)** Assume that W is a weight given to the current node.
- (Step 3)** Equally distribute weights to the lower nodes of the current node so that the total is $W/2$.

Two tree structures are compared in order from the root node to check conformity of both nodes as shown in Fig.3. The distance, $\text{Distance}(\text{root}_i, \text{root}_k)$, is initialized as zero. When different nodes are found in the conformity comparison, the weight of that node is added to the distance. The lower nodes below this node are all ignored. Especially, when

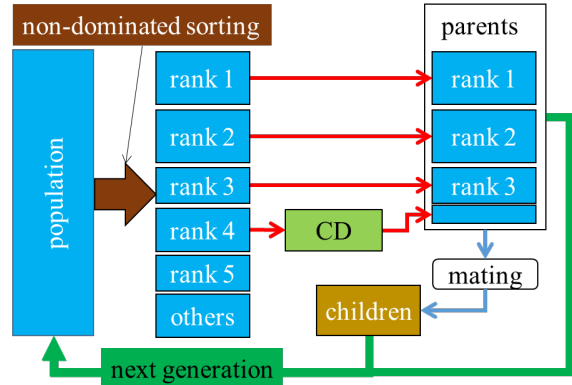


Figure 4: Conventional NSGA-II with CD.

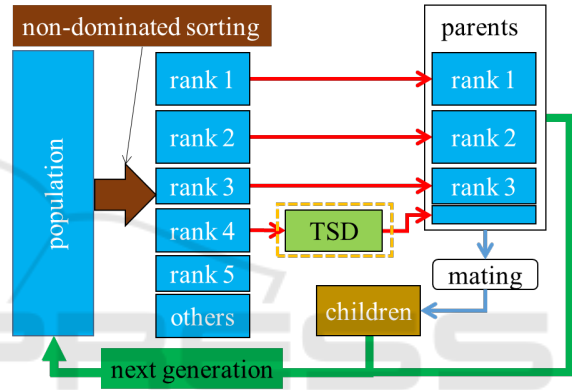


Figure 5: Modified NSGA-II with tree-structural distance.

the tree structures of both are completely different, $\text{Distance}(\text{root}_i, \text{root}_k)$ is given 1 as the maximum value.

Now, we have defined the three-objective optimization problem. NSGA-II shown in Fig.4 is applied to solve this problem. NSGA-II selects parent individuals by using non-dominated sorting and ranking with CD. Since tree-structure data is to be optimized in this paper, CD based only on the value of the objective function does not necessarily bring the diversity of the tree structure. Therefore, this paper propose to use TSD when selecting parents from the rank set overflowing from the parent group. A block chart of the modified NSGA-II with TSD is shown in Fig.5.

4 DOUBLE SPIRAL PROBLEM

A double spiral problem is applied to verify an effectiveness of the proposed techniques. The double spiral problem is a problem of classifying two data sets arranged in a spiral shape, and it is known as a problem that is difficult to solve even using neural net-

works(De Bonet et al., 1997; Yang and Kao, 2000). These two data sets are arranged as shown in Fig.6 and are to be classified by the following function f .

$$\begin{cases} f(x,y) > 0 & \iff (x,y) \in \mathbf{D}_1, \\ f(x,y) < 0 & \iff (x,y) \in \mathbf{D}_2, \\ f(x,y) = 0 & \iff \text{FALSE}, \end{cases} \quad (6)$$

where (x,y) denotes the coordinates of each point on the two-dimensional plane, and \mathbf{D}_1 and \mathbf{D}_2 denote the data sets expressed with the red crosses and the blue circles shown in Fig.6 respectively. In this paper, the case when $f(x,y) = 0$ is treated as classification failure at the point (x,y) .

The following nodes are prepared as elements for constituting the classifying function f .
 -nonterminal nodes: $\{+, -, *, \div, \sin, \cos, \tan, \text{ifltz}\}$
 -terminal nodes: $\{x, y, \text{constant}\}$
 where ifltz denotes a function with three arguments representing a conditional branch as follows,

$$\begin{aligned} \text{ifltz}(a,b,c) &\triangleq \text{if } a < 0 \text{ then } b \text{ else } c, \\ &= \begin{cases} b & (a < 0), \\ c & (\text{otherwise}). \end{cases} \end{aligned} \quad (7)$$

In order to verify the effectiveness, the following four combinations are applied to the double spiral problem, combination of the conventional operators and CD (expressed as "CO+MU & CD"), combination of the conventional operators and TSD (expressed as "CO+MU & TSD"), combination of PS operator and CD (expressed as "PS & CD") and combination of PS operator and TSD (expressed as "PS & TSD"). The conventional operators denotes

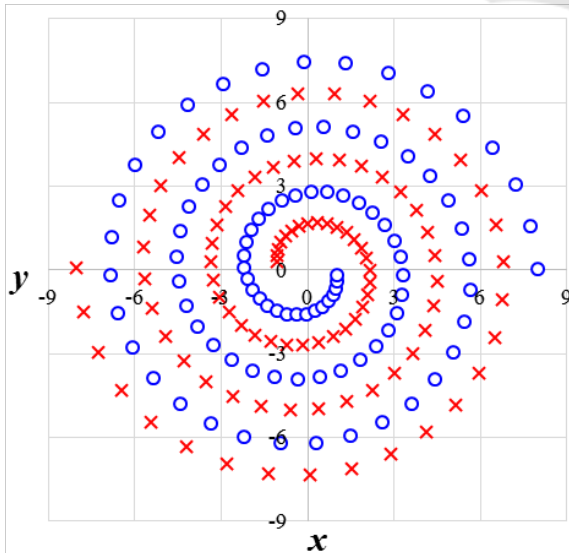


Figure 6: Arrangement of two data sets for double spiral problem. The red cross denotes a point in the class \mathbf{D}_1 and the blue circle denotes a point in the class \mathbf{D}_2 .

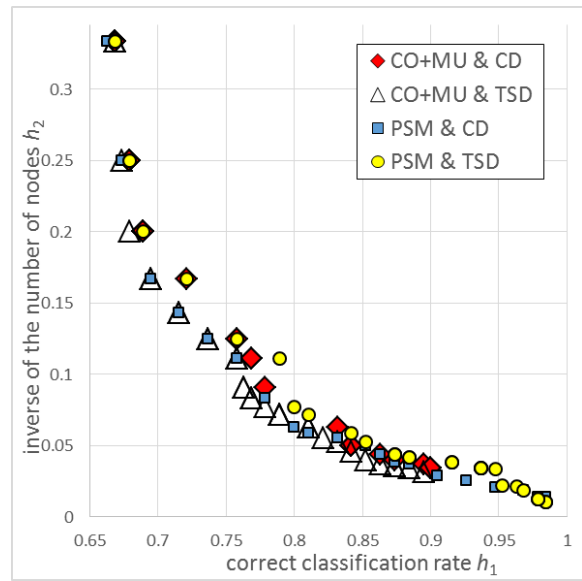


Figure 7: Distribution on the h_2-h_1 plane of the first front set in the final generation when using each method.

the conventional crossover and the conventional mutations(Koza, 1992; Koza, 1994; Ito et al., 1998; Sawada and Kano, 2003). The size of the population, the running generations, the number of points in the double spiral problem are defined as 100, 1,000,000 and 190 respectively. The probability, p_{met} , for selecting the type of the metastasis is set to 0.5, 0.25 and 0.75.

Fig.7 shows distributions on the h_2-h_1 plane of the first-front set in the final generation. As shown by Fig.7, NSGA-II with combining PS operator and TSD has given the best solution set, distributed in the upper right direction, in the widest range. The solutions obtained by NSGA-II with combining PS operator and CD has relatively high diversity but their evaluations are not so good. NSGA-II with combining the conventional operators and CD has given relatively good solutions but their diversity is low. NSGA-II with combining the conventional operators and TSD has given the worst solution set with the lowest diversity.

Fig.8 shows a comparison of distribution on the h_2-h_1 plane of the first front set in the final generation when 3-objective and 2-objective optimizations are executed by using the PS operator with $p_{\text{met}} = 0.50$ and TSD for the ranking. Compared to the distribution of solutions given by 2-objective optimization, the 3-objective optimization has acquired far better solutions in wider range. When PS operator with $p_{\text{met}} = 0.50$ and CD are combined, the same result has been obtained as shown in Fig.9. This shows an effectiveness of multi-objective optimization of the tree-structure data as proposed in this paper.

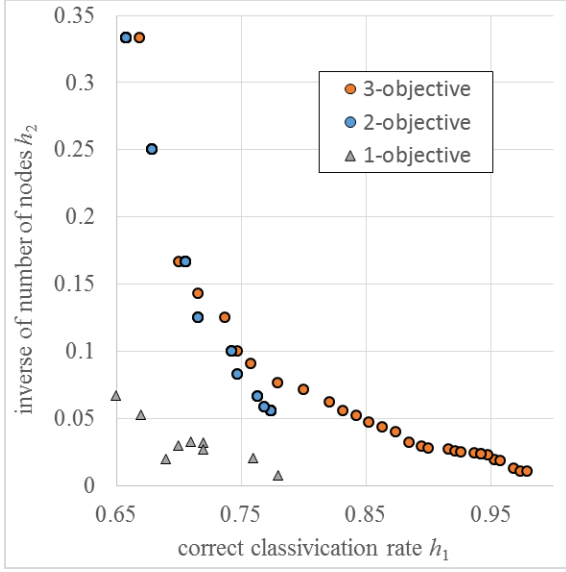


Figure 8: Comparison of distribution on the h_2 - h_1 plane of the first front set in the final generation when 3-objective and 2-objective optimizations are executed by using the PS operator with $p_{met} = 0.50$ and TSD for the ranking.

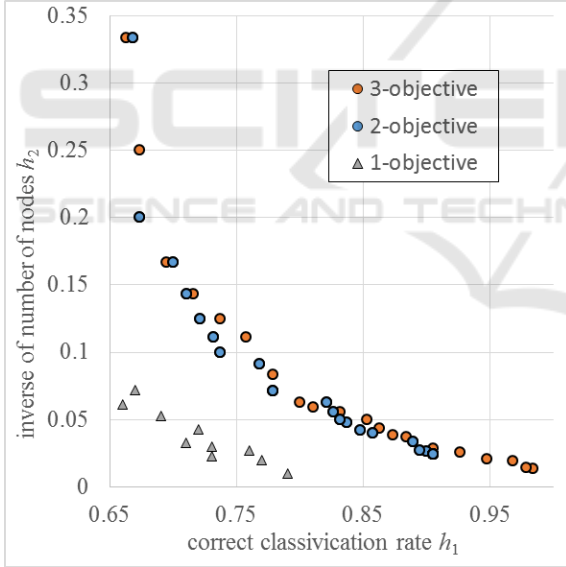


Figure 9: Comparison of distribution on the h_2 - h_1 plane of the first front set in the final generation when 3-objective and 2-objective optimizations are executed by using the PS operator with $p_{met} = 0.50$ and CD for the ranking.

Norm (Sato et al., 2006) and Maximum Spread (MS)(Zitzler, 1999) are applied for evaluation of each method. Norm denotes a measure of the convergence of the population to the Pareto front \mathcal{PF} and is defined by the following equation.

$$\text{Norm}(\mathcal{PF}) = \frac{1}{|\mathcal{PF}|} \sum_{j=1}^{|\mathcal{PF}|} \sqrt{\sum_{i=1}^m f_i(\mathbf{x}_j)^2}, \quad (8)$$

Table 1: Values of Norm and MS as a result of three-objective optimization given by each method. CO+MU denotes the conventional crossover operator and the conventional mutation operators. PS denotes PS operator.

operator	ranking	Norm	MS
CO+MU	CD	0.820	1.110
	TSD	0.795	1.100
PS $p_{\alpha} = 0.25$	CD	0.835	1.125
	TSD	0.835	1.125
PS $p_{\alpha} = 0.50$	CD	0.845	1.130
	TSD	0.865	1.140
PS $p_{\alpha} = 0.75$	CD	0.825	1.110
	TSD	0.850	1.140

where \mathbf{x}_j denotes the j -th individual of the Pareto front \mathcal{PF} . The larger the Norm value, the closer the approximate Pareto front \mathcal{PF} . MS denotes a measure of the spread of the first front at the final generation (Zitzler, 1999) and is defined by the following equation.

$$\text{MS}(\mathcal{PF}) = \sqrt{\sum_{i=1}^m \left(\max_{j=1}^{|\mathcal{PF}|} f_i(\mathbf{x}_j) - \min_{j=1}^{|\mathcal{PF}|} f_i(\mathbf{x}_j) \right)^2}. \quad (9)$$

The larger the MS value, the wider the spread of the population given by the optimization.

Table 1 shows values of Norm and MS given by each method. CO+MU denotes when the conventional crossover operator and the conventional mutation operators are used for the mating, PS denotes PS operator, and $p_{met} = *$ denotes when PS operator with the metastasis selection probability, p_{met} , which is equal to $*$. $*$ is used for the mating. Fig.10 is a graphical representation of the contents of Table 1. In this figure, PS $*$ denotes when PS operator with the metastasis selection probability, p_{met} , which is equal to $*$. $*$ is used for the mating. Concerning both Norm and MS values, the best result has been obtained by the method using PS operator with $p_{met} = 0.50$ and TSD. The results using PS operator have gathered in the upper right of the figure, whereas the results using the conventional crossover and the conventional mutation have gathered in the lower left. This shows the superiority of PS operator. On the other hand, the advantage of TSD has not been clearly shown by this experiment. TSD have optimized relatively better only when combined with PS operator. NSGA-II even with TSD has given the worst results when combined with the conventional operators. The reason for this result is considered as that TSD has a low ability to preserve extreme solutions as CD does. In the case of the multi-objective optimization of the tree structure, the ability to retain the diversity of tree structures like the

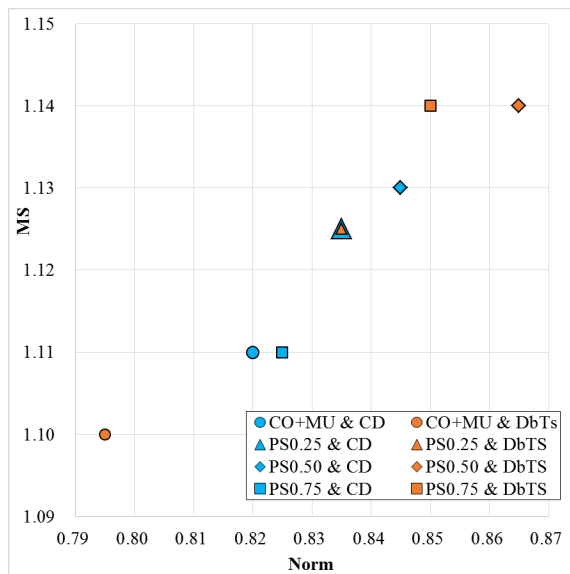


Figure 10: Comparison of results by each method on MS-Norm plane. CO+MU denotes when the conventional crossover operator and the conventional mutation operators are used for the mating. PS*. ** denotes when PS operator with the metastasis selection probability, p_{met} , which is equal to *. **, is used for the mating.

ranking with TSD is necessary, then an improvement to add ability to preserve the extreme solutions like CD should be considered.

5 CONCLUSION

In this paper, multi-objective optimization technique have been applied to the optimization of the tree-structure data, or GP. The size of the tree structure and the tree structural distance (TSD) are additionally introduced into the measure of the goodness of the tree structure as the objective functions. Furthermore, the partial sampling (PS) operator is proposed to effectively search the tree structure while avoiding bloat. In order to verify the effectiveness of the proposed techniques, they have applied to the double spiral problem.

By means of the multi-objective optimization of tree-structure data, we found that more diverse and better tree structures are acquired. The proposed method incorporating PS operator and TSD in NSGA-II has given relatively good results. However, since PS operator has low ability to numerically optimize constant nodes of the tree structure, it has not well worked effectively for the function optimization. In addition, since ranking with TSD in NSGA-II has low ability to preserve extreme solutions in the objective

function space, solutions not have been effectively selected.

In the future, a technique to incorporate numerical optimization ability such as a particle swarm optimization (Kenny, 1995) and the mutation to PS operator and the ranking selection technique combining TSD and CD should be considered in the future. The PS operator proposed in this paper has a mechanism to terminate the proliferation, but does not have no mechanism to forcibly exit from the PS operator. Such the mechanism to forcibly exit from the PS operator should be considered.

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