

Distributed Modified Extremal Optimization for Reducing Crossovers in Reconciliation Graph

Keiichi Tamura, Hajime Kitakami, and Akihiro Nakada

Abstract—To determine the mechanism of molecular evolution, a reconciliation graph is constructed from two heterogeneous trees, which are referred to as ordered trees. In the reconciliation graph, the leaf nodes of the two ordered trees face each other. Furthermore, leaf nodes with the same label name are connected to each other by an edge. To carry out reconciliation work efficiently, it is necessary to find the state with the minimum number of crossovers of edges between leaf nodes. Reducing crossovers in a reconciliation graph is a combinatorial optimization problem. In this paper, we propose a novel bio-inspired algorithm called distributed modified extremal optimization (DMEO). This algorithm is a hybrid of population-based modified extremal optimization (PMEO) and the distributed genetic algorithm model that is used for reducing crossovers in a reconciliation graph. We have evaluated DMEO using actual data sets. DMEO shows better performance compared with PMEO.

Index Terms—extremal optimization, distributed genetic algorithm, evolutionary computation, reconciliation graph

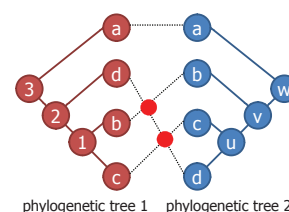
I. INTRODUCTION

MOLECULAR biologists need to carry out reconciliation work [1], [2], [3], [4] in order to determine the mechanism of molecular evolution. In reconciliation work, the relation between two heterogeneous phylogenetic trees and the relation between a phylogenetic tree and a taxonomic tree are compared. To compare two trees, we construct a graph called a reconciliation graph that consists of two phylogenetic trees or a phylogenetic tree and a taxonomic tree. Phylogenetic trees and taxonomic trees in a reconciliation graph are referred to as ordered trees. The leaf nodes of these ordered trees face each other. Moreover, leaf nodes with the same label name are connected to each other by an edge. To carry out reconciliation work efficiently, it is necessary to find the state with the minimum number of crossovers of edges between leaf nodes in the reconciliation graph.

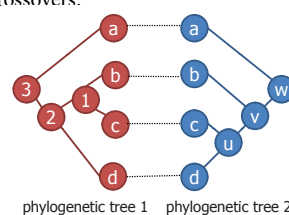
In Fig. 1, phylogenetic tree 1 and phylogenetic tree 2 are inferred from different molecular sequences with four identical species “a,” “b,” “c,” and “d.” The leaf nodes of phylogenetic tree 1 and those of phylogenetic tree 2 face each other. Leaf nodes representing the same species are connected to each other. The reconciliation graph shown in Fig. 1(a) has two crossovers. If we reduce crossovers in the reconciliation graph, we can obtain the reconciliation graph shown in Fig. 1(b), which has no crossovers.

Reducing crossovers in a reconciliation graph is a combinatorial optimization problem. The number of combinations increases exponentially as the number of leaf nodes increases. There are some heuristics [5], [6] that can be used for reducing crossovers in a reconciliation graph, and

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(a) Reconciliation graph with two crossovers.



(b) Reconciliation graph with no crossovers.

Fig. 1. Examples of reconciliation graphs ((a) shows a reconciliation graph that has two crossovers, and (b) shows a reconciliation graph that has no crossovers).

they use a genetic algorithm(GA)[7], extremal optimization (EO) [8], [9], [10], and modified EO (MEO)[11]. In our previous study[12], we proposed population-based modified extremal optimization (PMEO), which is a combination of a population-based approach and MEO.

PMEO shows better performance compared with MEO. However, it is difficult to maintain diversity at the end of alternation of generations. To overcome this difficulty, this paper proposes a novel extremal optimization model called distributed modified extremal optimization (DMEO) for reducing crossovers in a reconciliation graph. DMEO is a hybrid of PMEO and the distributed genetic algorithm (DGA) model [13], [14]. In the DGA model, we divide a population into two or more sub-populations and each sub-population evolves individually. Therefore, DMEO can maintain diversity at the end of alternation of generations.

The main contributions of this study are as follows:

- Distributed modified extremal optimization (DMEO) is proposed. DMEO is a hybrid bio-inspired algorithm that combine PMEO and DGA. Many studies [8], [9], [10], [15], [16], [17], [18] have applied EO to combinatorial optimization problems such as the traveling salesman problem, graph partitioning problem, and image rasterization. Recently, some studies [19], [20] have focused on integrating a population-based approach in EO. To the best of our knowledge, there is no study on population-based EO involving the use of the distributed genetic algorithm model.
- To evaluate the proposed DMEO, we implemented

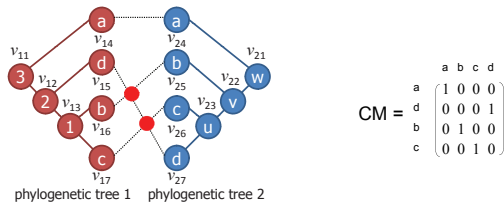


Fig. 2. Problem definition.

MDEO for reducing crossovers in a reconciliation graph. Moreover, we evaluated DMEO using two actual data sets for experiments. Experimental results shows that DMEO outperforms PME0.

The rest of the paper is organized as follows. Section II presents the problem definition. Section III explains PME0. Section IV proposes DME0. Section V presents experimental results, and Section VI concludes the paper.

II. PROBLEM DEFINITION

A reconciliation graph (RG) consists of two ordered trees, $OT_1 = (V_1, E_1)$ and $OT_2 = (V_2, E_2)$, where V_1 and V_2 are finite sets of nodes and E_1 and E_2 are finite sets of edges. A node that has no child nodes is a leaf node. The leaf node sets of OT_1 and OT_2 are denoted by $L_1 \in V_1$ and $L_2 \in V_2$, respectively. If the number of species is n , the number of leaf nodes is n . A leaf node has a label name, which is a species' name. The label name set is denoted by L_{leaf} .

In the reconciliation graph, OT_1 and OT_2 are located face to face. If a leaf node of OT_1 has the same label name as that of OT_2 , then the two leaf nodes are connected to each other. In Fig.2, phylogenetic tree 1 is OT_1 and phylogenetic tree 2 is OT_2 . The leaf node set L_1 has four nodes, v_{14} , v_{15} , v_{16} , and v_{17} . Similarly, L_2 has four nodes, v_{24} , v_{25} , v_{26} , and v_{27} . There are four label names in L_{leaf} , "a," "b," "c," and "d." Two leaf nodes v_{14} and v_{24} are connected because they have the same label name "a."

Let OL_1 and OL_2 be the order lists of leaf nodes:

$$OL_1 = [ol_{1,1}, ol_{1,2}, \dots, ol_{1,n}] (ol_{1,i} \in L_1, \mathcal{L}(ol_{1,i}) \in L_{leaf}),$$

$$OL_2 = [ol_{2,1}, ol_{2,2}, \dots, ol_{2,n}] (ol_{2,i} \in L_2, \mathcal{L}(ol_{2,i}) \in L_{leaf}),$$

where function \mathcal{L} returns the label name of an input node.

The function $C(M)$ returns the number of crossovers:

$$C(M) = \sum m_{j,\beta} m_{k,\alpha} [1 \leq j < k \leq n, 1 \leq \alpha < \beta \leq n], \quad (1)$$

where $m_{i,j}$ is (i, j) th-element of the connection matrix M that is defined as

$$m_{i,j} = \begin{cases} 1 & \text{if } \mathcal{L}(ol_{1,i}) = \mathcal{L}(ol_{2,j}), \\ 0 & \text{otherwise.} \end{cases} \quad (2)$$

In Fig. 2, OL_1 is given by $OL_1 = [v_{14}, v_{15}, v_{16}, v_{17}]$. Similarly, there are four leaf nodes in phylogenetic tree 2, $ol_{2,1} = v_{24}$, $ol_{2,2} = v_{25}$, $ol_{2,3} = v_{26}$, and $ol_{2,4} = v_{27}$. Therefore OL_2 is given by $OL_2 = [v_{24}, v_{25}, v_{26}, v_{27}]$. Fig. 2 also shows M . For example, the $(0, 0)$ th-element $m_{0,0}$ is 1 because $\mathcal{L}(v_{14})$ equals $\mathcal{L}(v_{24})$. Similarly, the $(1, 1)$ th-element $m_{1,1}$ is 0 because $\mathcal{L}(v_{15})$ does not equal $\mathcal{L}(v_{25})$.

The task of reducing crossovers in the reconciliation graph is defined as follows:

$$\begin{aligned} \min : & C(M), \\ \text{subject to :} & (1) M \text{ is the connection matrix of the } RG, \\ & (2) \text{ There are no crossovers on edges} \\ & \text{between non-leaf nodes in the } RG. \end{aligned}$$

There should be no crossovers on edges between non-leaf nodes in the reconciliation graph. For this constraint, we need to change order of leaf nodes by changing the order of child nodes in intermediate nodes. We cannot change the order between v_{15} and v_{17} (Fig. 2) because it will lead to the presence of crossovers on edges between non-leaf nodes. If we want to change the order between v_{15} and v_{17} , it is necessary to replace v_{15} and v_{13} , which are child nodes of v_{12} . If we replace v_{15} and v_{13} , the number of crossovers in the reconciliation graph becomes zero, and OL_1 is changed to $OL_1 = [v_{14}, v_{16}, v_{17}, v_{15}]$.

III. POPULATION-BASED MODIFIED EXTREMAL OPTIMIZATION

EO[8], [9], [10] follows the spirit of the Bak-Sneppen model, updating variables that have one of the worst values in a solution and replacing them by random values without ever explicitly improving them. EO divides an individual I into n components O_i ($1 \leq i \leq n$). Let λ_i be the fitness value of O_i . First, EO selects O_{worst} , which has the worst fitness value. Second, the state of component O_{worst} is changed at random. Henceforth, selection and change state of a component are repeated. The component with the worst fitness value has a high possibility that the fitness value of it will become better by changing state. Consequently, the fitness value of the individual also gets better because the fitness value of the component with worst fitness value gets better.

Modified EO (MEO) [11] generates two or more neighbor individuals as candidates for the next generation individual. The best neighbor individual among the candidates is selected as the next generation individual. Moreover, MEO uses roulette selection to select a component. First, MEO selects $O_{selected}$ with roulette selection. The selection rates of roulette selection are reciprocals of fitness values with components. Second, MEO generates new individual I' from I by changing the state of $O_{selected}$. Third, the generated I' is stored into $Candidates$. Finally, MEO selects the best individual from $Candidates$.

Population-based MEO (PME0) [12] involves a population-based approach. There are two or more individuals in a population. Alternation of generation is repeatedly performed for every individual by using MEO. To improve the search efficiency, individuals copy a sub-structure of an individual that has good sub-structures at each alternation of generations. This operation resembles the crossover operation in genetic programming (GP). However, one side only copies a sub-structure of another side. Copying of good sub-structures leads to a high probability of generation of a good individual. As a result, efficient search can be performed by maintaining diversity.

IV. DISTRIBUTED MODIFIED EXTREMAL OPTIMIZATION

This section explains the main concept of DME0 and the algorithm of DME0 for reducing crossovers in a reconciliation graph.

A. Main Concept

DMEO is a hybrid of PME0 and DGA model. DME0 divides the entire population into two or more sub-populations. A sub-population evolves individually by PME0. Moreover, from each sub-population, some individuals are selected and transferred to another sub-population. In return, the same number of migrants are received from another sub-population. DME0 repeats the following two steps:

- (1) Sub-populations should be made to evolve through one or more generations by using PME0.
- (2) Some individuals of a sub-population are migrated to another sub-population.

Each sub-population evolves individually. Each sub-population converges to the separate best solution. Therefore, DME0 can maintain diversity at the end of alternation of generations.

B. Definition of Individual and Component

A reconciliation graph is defined as an individual. A component of an individual is defined as a pair of leaf nodes with the same label name:

$$O_i = \{ol_{1,i}, ol_{2,\delta(i)}\} \quad (\mathcal{L}(ol_{1,i}) = \mathcal{L}(ol_{2,\delta(i)})). \quad (3)$$

Let $ol_{1,i}$ be a leaf node of OL_1 and $ol_{2,\delta(i)}$ be a leaf node of OL_2 . The function $\delta(i)$ returns the subscript number of an element of OL_2 whose label name is the same as the label name of $ol_{1,i}$. To change the state of O_i , it is necessary to change the order of child nodes of ancestor nodes of $ol_{1,i}$ or $ol_{2,\delta(i)}$. Here, $\mathcal{AS}(T, lname)$ is a set of ancestor nodes of a leaf node in T that has the label name $lname$.

The number of crossovers between $ol_{1,i}$ and $ol_{2,\delta(i)}$ is denoted by $\mathcal{C}(M, i)$. The following are the definitions of $\mathcal{C}(M, i)$ and the fitness value λ_i of O_i :

$$\lambda_i = \frac{\mathcal{C}(M) - \mathcal{C}(M, i)}{\mathcal{C}(M)}, \quad (4)$$

$$\mathcal{C}(M, i) = \sum_{l=i+1}^n \sum_{m=1}^{\delta(i)-1} \frac{m_{l,m}}{2} + \sum_{l=1}^{i-1} \sum_{m=\delta(i)+1}^n \frac{m_{l,m}}{2}. \quad (5)$$

In Fig. 2, there are four components, $O_1 = \{ol_{1,1}, ol_{2,1}\} (= \{v_{14}, v_{24}\})$, $O_2 = \{ol_{1,2}, ol_{2,4}\} (= \{v_{15}, v_{27}\})$, $O_3 = \{ol_{1,3}, ol_{2,2}\} (= \{v_{16}, v_{25}\})$, and $O_4 = \{ol_{1,4}, ol_{2,3}\} (= \{v_{17}, v_{26}\})$, with $\delta(1) = 1$, $\delta(2) = 4$, $\delta(3) = 2$, and $\delta(4) = 3$. The fitness values of the components are $\lambda_1 = 1$, $\lambda_2 = 1/2$, $\lambda_3 = 3/4$, and $\lambda_4 = 3/4$.

C. Algorithm

The algorithm of DME0 for reducing crossovers in a reconciliation graph consists of two steps: (1) Evolution Step and (2) Migration Step (Algorithm 1). First, an initial population divided to p sub-populations (p is the number of sub-populations). In the Evolution Step (step 5), all sub-populations are made to evolve through m generations by using the function $\mathbf{PME0}(SubP_i, m)$ (m is migration interval). In Migration Step (step 6), some individuals of a sub-population are migrated to another sub-population. Finally, the best individual from all sub-populations (step 7 and step 8).

Algorithm 1 DME0

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1: Generate initial population  $P_{init}$  at random.
2:  $I_{best} \leftarrow \mathbf{BEST}(P_{init})$ 
3: Divide  $P_{init}$  into  $p$  sub-populations  $SubP_i$ .
4: for  $i = 1$  to  $max\_generations/m$  do
5:   (Evolution Step) For all sub-populations, sub-
     population  $SubP_i$  should be made to evolve
     through  $m$  generations by using the function
      $\mathbf{PME0}(SubP_i, m)$ .
6:   (Migration Step) For all sub-populations, migrate
     some individuals of a sub-population to another sub-
     population.
7:   if  $\mathbf{F}(\mathbf{BEST}(SubP_1 \cap \dots \cap SubP_p)) > \mathbf{F}(I_{best})$  then
8:      $I_{best} \leftarrow \mathbf{BEST}(SubP_1 \cap \dots \cap SubP_p)$ 
9:   end if
10: end for

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Algorithm 2 PME0(P, m)

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1: for  $i = 1$  to  $m$  do
2:   for all  $I \in P$  do
3:     Evaluate fitness value  $\lambda_i$  of each component  $O_i$  of
      $I$ .
4:      $C \leftarrow \phi$ 
5:      $n \leftarrow 0$ 
6:     while  $n < num\_of\_candidates$  do
7:       Select  $O_{selected}$  by roulette selection (selection
       rates are the reciprocal of fitness values with
       components).
8:        $C \leftarrow C \cup \mathbf{GNI}(I, O_{selected})$ 
9:        $n \leftarrow n + 1$ 
10:    end while
11:     $I \leftarrow \mathbf{BEST}(C)$ 
12:  end for
13:   $\mathbf{CSS}(P)$ 
14: end for

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D. Evolution Step

In the Evolution Step, all sub-populations are made to evolve through m generations by using the function $\mathbf{PME0}$ (Algorithm 2). First, for each individual, the state of the individuals in P is changed by using MEO. Second, the function \mathbf{CSS} copies a good sub-structure of an individual to another individual.

In the MEO steps, for each individual, the following steps are executed. Initially, the function evaluates the fitness value λ_i (step 3). Next, the following three steps are repeated while n is less than $num_of_candidates$. First, component $O_{selected}$ in I is selected by using the roulette selection (step 7). Second, the function generates a neighbor individual from I with the function \mathbf{GNI} . The function \mathbf{GNI} generates a neighbor individual by changing the state of component $O_{selected}$. Third, the neighbor individual is stored in C (step 8). Finally, the best individual in C is selected and I is replaced by it (step 11).

The state of $O_{selected}$ is changed by changing the order of child nodes in an intermediate node that is an ancestor node of $O_{selected}$. The processing steps of \mathbf{GNI} are as follows. First, the outputs of $\mathcal{AS}(T_1, \mathcal{L}(O_{selected}))$ or $\mathcal{AS}(T_2, \mathcal{L}(O_{selected}))$ are stored in the set $Ancestors$. Then,

TABLE I
DATA SETS

	Taxonomic tree		Phylogenetic tree	
	Number of nodes	Number of leaf nodes	Number of nodes	Number of leaf nodes
<i>Housekeeping</i>	241	40	79	40
<i>Moss</i>	290	207	394	207

Algorithm 3 CSS(P)

```

1: Select individual  $SI \in P$  by roulette selection (selection
   rates are the fitness values of components).
2: for all  $I \in P, I \neq SI$  do
3:   for  $i = 1$  to  $n$  do
4:     Calculate the difference  $diff_i$  between the fitness
       value of  $O_i$  in  $SI$  and the fitness value of  $O_j$  in  $I$ ,
       where  $O_i$  and  $O_j$  have the same label name.
5:   end for
6:   Select  $O_{selected}$  by roulette selection (selection rates
   are  $diff_i$ ).
7:    $A \leftarrow \mathcal{AS}(T_1, \mathcal{L}(O_{selected}))$  or  $\mathcal{AS}(T_2, \mathcal{L}(O_{selected}))$ 
8:    $C \leftarrow \phi$ 
9:   for all  $a \in A$  do
10:    Generate a new individual  $I'$  from  $I$  by changing
       the order of child nodes in  $a$ .
11:     $C \leftarrow C \cup I'$ 
12:   end for
13:    $I \leftarrow \text{BEST}(C)$ 
14: end for

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node a is selected at random from A . Finally, the order of the child nodes in a is changed. Suppose that the selected component is O_2 in Fig. 2. The function $\mathcal{AS}(T_1, \mathcal{L}(O_2))$ returns $\{v_{12}, v_{11}\}$ and $\mathcal{AS}(T_2, \mathcal{L}(L_2))$ returns $\{v_{22}, v_{21}\}$. If $Ancestors = \{v_{12}, v_{11}\}$ and v_{12} is selected as a , the order of child nodes in v_{12} is changed. In this case, order of node v_{15} and v_{13} are changed. As a result, a new individual I' is obtained by the change of state.

Algorithm 3 shows the function CSS. At the beginning, an individual SI in P is selected by roulette selection (step 1). Each individual of P copies a sub-structure of SI by the following steps. First, the function calculates the difference $diff_i$ between the fitness value of O_i of SI and the fitness value of O_j of I , where O_i and O_j have the same label name (steps 3, 4, and 5). Second, $O_{selected}$ is selected by roulette selection (step 6). Next, $\mathcal{AS}(T_1, \mathcal{L}(O_{selected}))$ or $\mathcal{AS}(T_2, \mathcal{L}(O_{selected}))$ is stored in A (step 7). Then, for all $a \in A$, a new individual I' is generated from I by changing the order of child nodes in a , and I' is stored in C (steps 9, 10, 11, and 12). Finally, the function selects the best individual from C (step 13).

E. Migration Step

In the Migration Step, some individuals of a sub-population are migrated to another sub-population. The distributed genetic algorithm model requires *number of sub-populations*, *migration rate*, *migration interval*, and *migration model*. The first three items are user-given parameters. The last item consists of two things: *selection method* and *topology*. The method used for the selection of individuals for migration is referred as

selection method. The structure of the migration of individuals between sub-populations is referred as *topology*. In this study, we use uniform random selection as the *selection method*. Moreover, the proposed algorithm uses the random ring migration topology. The most basic migration topology is the ring migration topology. In this topology, individuals are transferred between directionally adjacent sub-populations. In the random ring migration topology, an arrival sub-population to which individuals are to be migrated is decided at random.

V. PERFORMANCE EVALUATION

We performed four experiments for evaluating the performance of DMEO. In the experiments, the two data sets listed in Table I are used. The *Housekeeping* data set consists of a phylogenetic tree of the housekeeping gene and its taxonomic tree. The *Moss* data set consists of a phylogenetic tree of the rps4 gene and its taxonomic tree. The number of species in the *Housekeeping* data set is 40 and that in the *Moss* data set is 207.

Experiment 1 measured the number of crossovers of the best individual at each generation to compare DMEO and PME0. Experiment 2 also measured the number of crossovers of the best individual at each elapsed time to compare DMEO and PME0. Experiment 3 measured frequency of the number of crossovers of best individuals in fixed generations. Experiment 4 measured the number of crossovers of the best individual at each generation by changing the number of sub-populations.

In PME0 and DME0, the number of individuals in the population was set to 100. The user parameter *num_of_candidates* was set to 100 and m was set to 10000 in PME0. In DME0, the user parameter *num_of_candidates*, *migration_interval(m)*, *number of sub-populations(p)*, and *migration rate* were set to be 100, 10, 5 and 0.05, respectively. The number of individuals in a sub-population is 20. The number of crossovers was the average of three trials.

Experiment 1

In Experiment 1, we measured the number of crossovers of the best individual in each generation. Figure3(a) and Figure3(b) show the number of crossovers (vertical axis: the number of crossovers, horizontal axis: generations). Fig. 3(a) and Fig. 3(b) show that the number of crossovers of DME0 in each generation was smaller than that in the case of PME0. DME0 showed better performance compared with PME0.

The number of crossovers in PME0 is converging into around 300 when we use *Moss* data set. On the other hand, in DME0, the number of crossovers is converging into around 250. The diversity of PME0 is small, because the number of sub-populations is one. Therefore, the fitness

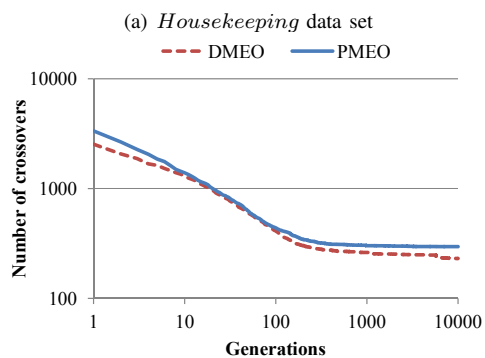
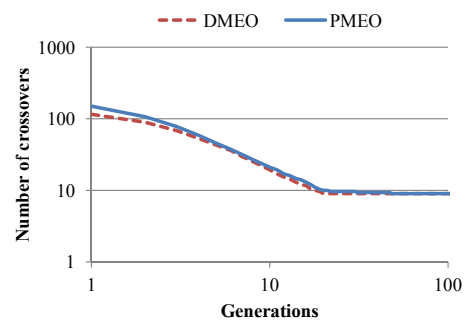


Fig. 3. Experiment 1 ((a) and (b) shows the number of crossovers of the best individual) .

value of a individual will not be improved in the end of alternation of generations.

Experiment 2

In Experiment 2, we measured the number of crossovers of the best individual at different time instants. The computation time of DME0 was longer than that in the case of PME0 because the former included the Migration Step. Therefore, it was necessary to compare the number of crossovers for the same computation time.

Fig. 4(a) and Fig. 4(b) show the number of crossovers at different time instants (vertical axis: the number of crossovers, horizontal axis: processing time). The number of crossovers of DME0 becomes smaller than that of PME0 at the end of alternation of generations.

Experiment 3

The number of crossovers of the best individual was measured 100 times for the 10,000th alternation generation. Figure 5(a) and Figure 5(b) show frequency of the number of crossovers when *Housekeeping* data set is used. The number of crossovers of the optimal solution of *Housekeeping* data set is 9. Both of them can obtain the best solution by 100%. Fig. 6(a) and Fig. 6(b) show the frequency of the number of crossovers for the *Moss* data set. In DME0, all the numbers of crossovers of optimal solutions were between 200 and 299. On the other hand, they were distributed between 200 and 400 for PME0. Above all, although 90% of optimal solutions were between 200 and 249 in the case of DME0, only a few optimal solutions were obtained between 200 and 249 in the case of MEO.

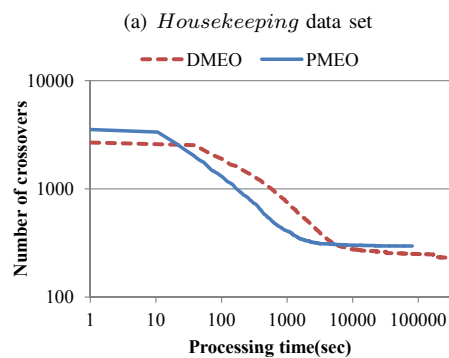
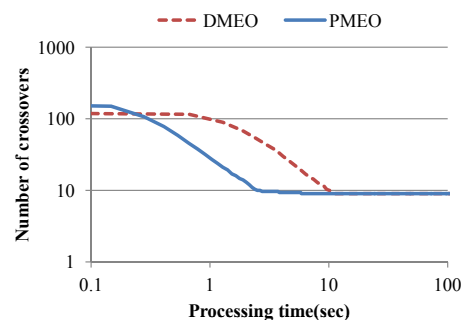


Fig. 4. Experiment 2 ((a) and (b) shows the number of crossovers of the best individual).

Experiment 4

In Experiment 4, we changed the number of sub-populations in DME0. Fig. 7 shows the results of Experiment 4 using *Moss* data set. When the number of sub-populations is four, it has fallen into the local optimal solutions. On the other hand, when the number of sub-populations is five or ten, convergence is not early. Therefore, they can obtain better solutions.

VI. CONCLUSION

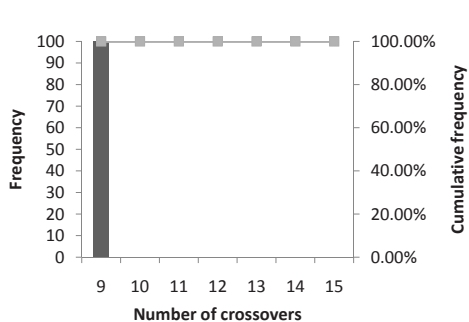
This paper proposes distributed modified extremal optimization (DME0) for reducing crossovers in a reconciliation graph. The proposed algorithm is a bio-inspired algorithm of population-based modified extremal optimization (PME0) and the distributed genetic algorithm model. We have evaluated DME0 by using actual data sets. Experimental results show that DME0 is better performance compared with PME0. In the future work, we will develop extended DME0 for making it applicable to other combination optimization problems.

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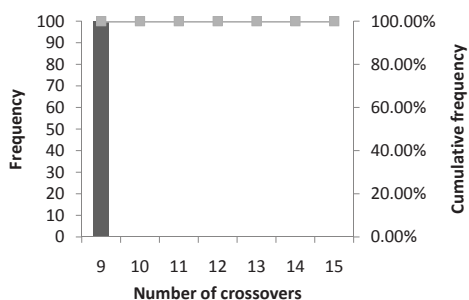
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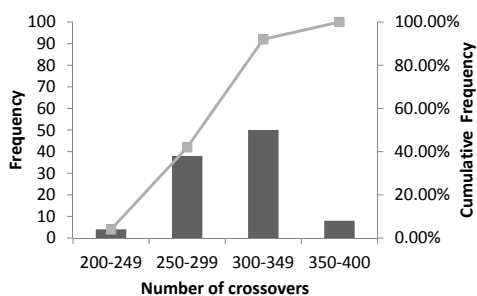


(a) PMEO

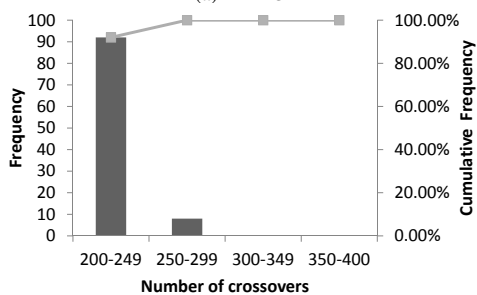


(b) DMEO

Fig. 5. Experiment 3 (*Housekeeping* data set).



(a) PMEO



(b) DMEO

Fig. 6. Experiment 3 (*Moss* data set).

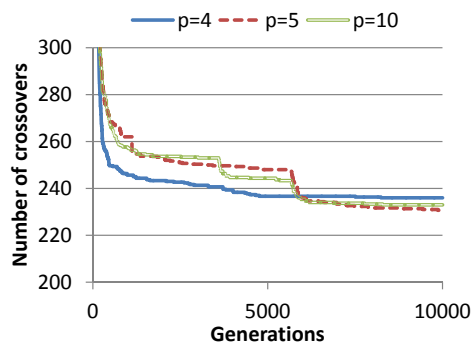


Fig. 7. Experiment 4 (*Moss* data set).

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