# Seeking Multiple Solutions of Combinatorial Optimization Problems: A Proof of Principle Study

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Abstract—Problems with multiple optimal solutions widely exist in the real world. In some applications, it is required to locate multiple optima. However, most studies are dedicated to the continuous multi-solution optimization, while few works contribute to the discrete multi-solution optimization. To promote the multi-solution research in the discrete area, we design a benchmark test suite for multi-solution traveling salesman problems and propose two evaluation indicators. Further, in order to solve the problems, the genetic algorithm is incorporated with a niching technique defined in the discrete space. The proposed algorithm is compared with an existing algorithm outperforms the compared algorithm concerning the quality and diversity of obtained solutions.

Keywords—multi-solution traveling salesman problem, multimodal optimization, genetic algorithm, neighborhood-based niching strategy

# I. INTRODUCTION

Combinatorial Optimization Problems (COPs) are a class of discrete optimization problems that need to find an optimal solution in a finite solution space according to some selection criteria. Many COPs are known to be NP-hard, such as the Traveling Salesman Problem (TSP). It is quite difficult to solve them by deterministic algorithms, especially when the solution space is large. In the past decades, many evolutionary algorithms (EAs) have been successfully developed to solve COPs [1-4], owing to their non-deterministic search characteristic and powerful global optimization ability. However, most studies focus on locating one single optimal solution. But many practical applications require to identify more than one optimal solution, such as the navigation system and the robot path planning. With a diverse solution set, the decision makers can choose the most proper one according to their preferences, or they can have alternatives in case of some unexpected situations.

The area of finding multiple optima for a single problem is generally known as multimodal optimization (MMO) or multi-solution optimization, which has undergone intensive studies in the past few years [5-8]. However, most studies are conducted on the continuous MMO, whereas seldom research is devoted to the discrete MMO. To extend the MMO to the discrete optimization area, there are three main issues required to be considered: (1) the baseline algorithms that are suitable to deal with discrete MMO problems; (2) the techniques to maintain multiple potential solutions in the discrete problem space; (3) an appropriate benchmark test suite. The first two are mainly considered by optimizer developers, while the third one is a crucial factor for evaluating the algorithm performance. In this paper, we conduct a proof of principle study for addressing these three issues, which are briefly introduced as follows.

The first issue regards the choice of an appropriate baseline algorithm for encoding and evolving solutions in the discrete problem space. Some EAs, such as Differential Evolution [9], Particle Swarm Optimization [10], and I-Ching divination EA [11, 12], use floating-point encoding by nature, and hence they cannot solve discrete problems directly. Other EAs, such as Genetic Algorithm (GA) [13, 14] and Ant Colony Optimization [15], are more suitable to use an integer encoding scheme and then work in the discrete or combinatorial space. Therefore, in this work, we choose GA as our baseline algorithm. However, GA cannot solve discrete MMO problems directly because it will converge towards an optimum eventually. The convergence is caused by the diversity loss.

Thus, the second issue focuses on preserving the population diversity, which is crucial for the MMO. In the continuous MMO, the primary methods to preserve population diversity are niching techniques, such as crowding [16, 17], speciation [18], and neighborhood strategy [5]. Niching techniques limit solutions evolving within the local space, which avoids the global convergence. Along this light of consideration, we can incorporate the niching strategies into a suitable baseline algorithm to obtain diverse candidates simultaneously. Specifically, we develop a neighborhood-based niching strategy into GA to deal with discrete MMO problems.

The third issue concerns the selection of the benchmark suite of discrete MMO problems. Although the multisolution optimization of COPs is critical for many practical applications, currently this area has received seldom attention and lacked a standard test suite to evaluate the related algorithms. The lack of an appropriate benchmark test suite may hinder the research and development for the discrete MMO area. To promote the development of this area, in this paper, we develop a benchmark test suite for the combinatorial MMO. Because TSP is the most popular and representative COP, we take it as an example and design a set of multi-solution TSP instances (MSTSPs). To our best knowledge, there are several early MSTSP instances have been reported [19, 20]. However, these instances either contain too many optimal tours (e.g., 16 cities with 938 optima) or possess a small number of cities (fewer than 10

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cities), which are inappropriate and insufficient to be utilized as a benchmark test suite. In this paper, we propose a benchmark suite with 25 MSTSP instances that are classified into three categories, i.e., the simple MSTSPs, the geometry MSTSPs, and the composite MSTSPs. The number of cities ranges from 9 to 66, and the number of optima scales from 2 to 196.

The rest of this paper is organized as follows. Section II formulates TSP. Section III describes the proposed 25 MSTSPs. The proposed algorithm is presented in Section IV. Section V defines the experimental settings and reports experimental results. Finally, the conclusion is drawn in Section VI.

#### II. TRAVELING SALESMAN PROBLEM

Given a number of cities and the distance information between each pair of them, a salesman visits each city only once to construct a Hamilton path. The target of TSP is to find the shortest Hamilton path. Mathematically, consider a graph G = (V, E), where  $V = \{1, 2, 3, ..., N\}$  is a set of cities (denoted by the indices), and  $E = \{(i, j) \mid i, j \in N, i \neq j\}$  is a set of edges indicating the connection between cities *i* and *j*. Each connection (i, j) has a weight value  $d_{ij}$  to measure the distance between the two cities. Following the edge weight type EUC\_2D defined in [21], we round the distance to the nearest integer.

The Hamilton path can be formulated as a permutation  $\pi$  for the city set. Thereafter, TSP is to find a shortest path in all permutations. More precisely, we consider

$$\min f(\pi) = \sum_{k=1}^{N-1} d_{\pi(k)\pi(k+1)} + d_{\pi(N)\pi(1)}$$
(1)

where *N* is the number of cities and  $\pi(k)$  is the *k*th element of the permutation  $\pi$ .

# **III. SUMMARY OF THE TEST SUITE**

Our benchmark set includes 25 MSTSPs. They are divided into three categories based on their design methods, which are generally described below.

The first category (MSTSP1 - MSTSP6) consists of six simple MSTSPs, whose cities are randomly generated. For these instances, we obtain the ground-truth best solutions by the brute-force search. However, since the solution space increases exponentially with the increasing number of cities, for relatively large-scale instances, it is impossible to traverse all possible permutations considering the time limitation. Consequently, in this category, the number of cities ranges from 9 to 12. Besides, the number of optima ranges from 2 to 13. As an example, the MSTSP1 are plotted in Fig. 1, where the black circles represent cities and the red lines constitute the optimal tour. Particularly, the MSTSP1 has three optimal tours, each has been depicted in a subgraph of Fig. 1. The length of each optimum is displayed above the subgraph. It can be observed that the three optima possess exactly the same length of 680, but different tours.

The second category (MSTSP7 - MSTSP12) includes six geometry MSTSPs. Unlike the first category that the instances are randomly generated, now we utilize the symmetrical geometry to construct MSTSPs. By designing different geometric topologies, these instances can have



Fig. 1.MSTSP1 with 9 cities and 3 optimal tours



Fig. 2.MSTSP9 with 10 cities and 4 optimal tours

diverse numbers of optima. Thus, in MSTSP7 - MSTSP12, the number of optima are between 4 and 196, while the number of cities are between 10 and 15. To be specific, different symmetrical geometries are used, including the rectangle, the regular pentagon, and the regular hexagon. Cities are located on vertexes of each geometry. Under different geometries, the optima have significantly different tours for each instance. We take MSTSP9 as an example, which is drawn in Fig. 2. A regular hexagon is nested inside a large rectangle, which generates four optimal tours. It can be observed from Fig. 2 that the four tours possess totally different topologies.

The third category (MSTSP13 - MSTSP25) is comprised of 13 composite MSTSPs, which are relatively large-scale instances. The composite MSTSPs are constructed with some basic small-scale MSTSPs. Each small-scale MSTSP is considered as a city cluster, and the city clusters are distributed at different geometric locations in the composite MSTSP. On the one hand, some city clusters possess diverse sub-tours with equal lengths, and thus provide multiple optimal tours for the composite MSTSPs. On the other hand, the geometric distribution of city clusters provides additional possibilities for the composite instances to have multiple diverse solutions. Thus, to summarize, the diversity of the optimal tours comes from both the intra-cluster relationship between cities and the inter-cluster relationship between city clusters. For MSTSP13 - MSTSP25, the maximum city size is raised to 66, while the number of optima ranges from 4 to 72. More specifically, the city clusters can be designed with geometric locations (such as the cases from MSTSP13 to MSTSP 16) or with randomly generated locations (such as the cases from MSTSP17 to MSTSP25). Moreover, concerning the inter-cluster relationship, MSTSP13 and MSTSP14 possess a single optimal tour for the city clusters, while the other composite MSTSPs have multiple optimal tours among city clusters. As an example, the MSTSP21 has two optimal inter-cluster topologies, which are shown in the two sub-figures of Fig. 3(a). Besides, the instance has four city clusters, which are labeled with A, B, C, and D, respectively, using a subscript with the index of the optimal topology. If we zoom in one of the city cluster (e.g., B<sub>1</sub>) to see more details, as shown in Fig. 3(b), the cluster has two different optimal intra-cluster topologies. Similarly, the cluster B<sub>2</sub>, displayed in Fig. 3 (c),

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Fig. 3.MSTSP9 with 48 cities and 4 optimal tours

possesses two distinct intra-cluster topologies with the equal subtour length.

The above three categories contain 25 MSTSPs in total, which are summarized in Table I, including the category information, the index, the name, the number of cities, the number of optima, and the optimal length. For more details, please refer to the supplementary file and the source code of the benchmark suite. They are available to download on the Internet <sup>1</sup>.

# IV. THE NEIGHBORHOOD-BASED GENETIC ALGORITHM

To settle the proposed 25 MSTSPs, a neighborhoodbased genetic algorithm (NGA) is proposed. GA is a popular optimizer to tackle TSP, for the easy implementation and good search ability. The neighborhood-based strategy restricts the search of neighborhood members within respective local spaces, allowing locating diverse candidate solutions simultaneously. Eventually, NGA can obtain various solutions at the end of optimization. In the following, we describe the details of NGA.

# A. Overall Framework

To begin with, NGA initializes *NP* chromosomes and evaluates their tour lengths. Next, the algorithm enters the evolution loop. The neighborhood strategy is adopted to divide the entire population into several groups and form a mating pool eventually. Then, pairwise parents in the mating pool execute partially mapped crossover (PMX) [23]. After that, we mutate the chromosomes by reversing genomes between two randomly selected positions, termed reverse sequence mutation (RSM) [24]. Thus far, we obtain offspring as well as their tour lengths. Afterwards, we select chromosomes from the offspring to determine the parents of

<sup>1</sup> https://github.com/GnauhGnit/MSTSP.

| Category  | Index   | Name #City #Optima |    | Optimal length |       |
|-----------|---------|--------------------|----|----------------|-------|
|           | MSTSP1  | simple1_9          | 9  | 3              | 680   |
|           | MSTSP2  | simple2_10         | 10 | 4              | 1265  |
| Circuit.  | MSTSP3  | simple3_10         | 10 | 13             | 832   |
| Shiple    | MSTSP4  | simple4_11         | 11 | 4              | 803   |
|           | MSTSP5  | simple5_12         | 12 | 2              | 754   |
|           | MSTSP6  | simple6_12         | 12 | 4              | 845   |
|           | MSTSP7  | geometry1_10       | 10 | 56             | 130   |
|           | MSTSP8  | geometry2_12       | 12 | 110            | 1344  |
| Constant  | MSTSP9  | geometry3_10       | 10 | 4              | 72    |
| Geometry  | MSTSP10 | geometry4_10       | 10 | 4              | 72    |
|           | MSTSP11 | geometry5_10       | 10 | 14             | 78    |
|           | MSTSP12 | geometry6_15       | 15 | 196            | 130   |
|           | MSTSP13 | composite1_28      | 28 | 70             | 3055  |
|           | MSTSP14 | composite2_34      | 34 | 16             | 3575  |
|           | MSTSP15 | composite3_22      | 22 | 72             | 9455  |
|           | MSTSP16 | composite4_33      | 33 | 64             | 8761  |
|           | MSTSP17 | composite5_35      | 35 | 10             | 9061  |
|           | MSTSP18 | composite6_39      | 39 | 20             | 23763 |
| Composite | MSTSP19 | composite7_42      | 42 | 20             | 14408 |
|           | MSTSP20 | composite8_45      | 45 | 20             | 10973 |
|           | MSTSP21 | composite9_48      | 48 | 4              | 6767  |
|           | MSTSP22 | composite10_55     | 55 | 9              | 10442 |
|           | MSTSP23 | composite11_59     | 59 | 10             | 24451 |
|           | MSTSP24 | composite12_60     | 60 | 36             | 9614  |
|           | MSTSP25 | composite13_66     | 66 | 26             | 9521  |

TEST INSTANCES OF MSTSPS

TABLE I.

# Algorithm 1 NGA

Input: A MMTSP test instance T, the population size NP, the neighborhood size m, the crossover rate  $P_c$ , the mutation ratio  $P_m$ , and the termination criterion.

Output: The representative solution set S.

- 1:  $Parent \leftarrow Initialize(NP)$
- 2: Evaluate(Parent)
- 3: While the termination criterion not satisfied do
- 4: *MatingPool* ← Neighborhood(*Parent*, m)
- 5: Offspring  $\leftarrow$  Crossover(MatingPool, "PMX") /\* apply the PMX [23] with a probability  $P_c */$
- 6: Offspring  $\leftarrow$  Mutation(Offspring, "RSM") /\* apply the RSM [24] with a probability  $P_m */$
- 7: Evaluate(Offspring)
- 8: *Parent*  $\leftarrow$  Selection(*Offspring, m*)
- 9: End While
- 10:  $S \leftarrow$  Preserve (*Parent*, *m*)

the next generation. The above procedures repeat until the termination condition is met. When the algorithm terminates, a post-processing method is applied to identify the representative solutions of the final populations and

| Algorithm | 2 Neighborhood(Parent | t, m) |
|-----------|-----------------------|-------|
|-----------|-----------------------|-------|

| Output: | The chromosome set MatingPool |
|---------|-------------------------------|
| 1.      | tmnParent ← Parent            |

- 2:  $MatingPool = \emptyset$
- 3: While *tmpParent*  $\neq \emptyset$  do
- 4: *Leader*  $\leftarrow$  FindBest(*tmpParent*)
- 5: CalculateShareDist(*tmpParent*, *Leader*)
- 6: *sortParent* ← Sort(*tmpParent*.shareDist, "ascending")
- 7:  $NeighborGroup \leftarrow sortParent [1, ..., m]$
- 8: If all the members of *NeighborGroup* are the same **then**
- 9: DiversityEnhancement(NeighborGroup)
- 10: End If
- 11: Shuffle(NeighborGroup)
- 12: MatingPool = MatingPool + NeighborGroup
- 13: *tmpParent = tmpParent NeighborGroup*
- 14: End While

output a solution set. The overall procedure is presented in Algorithm 1.

# B. Neighborhood Grouping Strategy

The neighborhood grouping strategy divides the entire population based on the individual distances. As presented in **Algorithm 2**, first, *tmpParent*, a copy of *Parent*, is created. Then, the chromosome with the shortest tour is identified as the neighborhood leader *Leader*. Subsequently, members who are close to *Leader* more tend to form a group. To this end, a similarity measure between solutions of MSTSPs is required.

Note that the solution of an MSTSP is encoded as a permutation, and hence it is meaningless to directly compare the city indexes on the corresponding positions. Instead, the adjacency information between cities is more important. Therefore, we define the similarity measure based on the common edges between two tours. Suppose  $\pi_i$  and  $\pi_j$  are two permutations, while  $\Phi(\pi_i)$  and  $\Phi(\pi_j)$  denote their edge sets. Then, the similarity between  $\pi_i$  and  $\pi_j$  is calculated as

$$S(\pi_i, \pi_j) = \frac{\left| \Phi(\pi_i) \cap \Phi(\pi_j) \right|}{N}$$
(2)

where  $|\cdot|$  denotes the number of edges in the intersection set.

After that, the similarity values between *Leader* and all members are calculated. The calculated values are used to sort *tmpParent* in an ascending order, obtaining *sortParent*. The first *m* chromosomes of *sortParent* together form *NeighborGroup*. In addition, we also consider the diversity loss caused by the trap of the local optima. A diversity enhancement approach is performed on *NeighborGroup* to avoid the search getting into the local optima. Specifically, if all the members of *NeighborGroup* are the same, we reinitialized *m*-1 members, leaving one member unchanged. Then, *NeighborGroup* are settled, they are added to *MatingPool*. In the meantime, the newly added members are eliminated from *tmpParent*. The above process is repeated until the set *tmpParent* is empty.

| Algorith | <b>m</b> 3 Preserve( <i>Parent</i> , <i>m</i> )                                      |
|----------|--|
| Output:  | The representative solution set $S$ .  |
| 1:       | ShortestLength SelectBestFitness(NeighborGroup) /* return the best fitness value. */ |
| 2:       | $thrLength \leftarrow ShortestLength \cdot (1 + \varepsilon)$                        |
| 3:       | $S = \emptyset$  |
| 4:       | For $i = 1$ to NP/m do   |
| 5:       | $NeighborGroup \leftarrow (Parent[(i-1)*m+1,, i*m])$                                 |
| 6:       | For every $e \in NeighborGroup$ do   |
| 7:       | If $\text{Exsit}(\mathcal{S}, e)$ then   |
| 8:       | continue   |
| 9:       | End If   |
| 10:      | If e.Length == ShortestLength then   |
| 11:      | $S \leftarrow S \cup s /*$ preserve the chromosome best                              |
|          | so far */  |
| 12:      | Else If $e$ .Length $\leq$ thrLength then  |
| 13:      | $maxSim \leftarrow 0$  |
| 14:      | For every $o \in S$ do   |
| 15:      | If $S(e, o) > maxSim$ then   |
| 16:      | $maxSim \leftarrow S(e, o)$  |
| 17:      | End If   |
| 18:      | End For  |
| 19:      | If <i>maxSim</i> < <i>thrSim</i> <b>then</b>   |
| 20:      | $S \leftarrow S \cup e$ /* preserve diverse  |
|          | chromosome*/   |
| 21:      | End If   |
| 22:      | End If   |
| 23:      | End For  |
| 24:      | End For  |
|          |  |

# C. Evolutionary Operations

The basic evolutionary operations of GA include crossover, mutation, and selection, which are shown in the lines 5 - 8 of **Algorithm 1**. The three operations are applied within the same neighborhood group to avoid global convergence. To be specific, crossover and mutation operations are adopted with parent pairs of the same neighborhood group. That is to say, most gene fragments of offspring are inherited from the members of the same neighborhood group, and hence the offspring and the parents tends to be close to each other. Selection operation keeps the superior and diverse solutions while discard the others. For each child, the most similar parent of the corresponding neighborhood group is identified. The length values between the child and this parent are compared. If the child is shorter, it will take the place of the chosen parent.

## D. Post-processing Method

When the algorithm terminates, it will obtain NP chromosomes, which correspond to NP solutions. However, some of them are unnecessarily to be provided because of redundancy or inferiority. Considering this, a post-processing method is called to identify the representative

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ones and then offer them in the final output set. The procedure is described in **Algorithm 3**. To begin with, find the solution with the shortest length and record the length as *ShortestLength*. Then, a selection threshold *thrLength* is defined as an  $\varepsilon$ -relaxion of the *ShortestLength*. Afterwards, we deal with the *NP* solutions one by one: we first check whether they have already existed in the final output set *S*. If yes, the redundant solutions will be discarded. Otherwise, we allow a solution to join *S* under two conditions: 1) its length is exactly the same as the length of so far optima (shown in the lines 10 - 11 of **Algorithm 3**), and 2) its length is shorter than *thrLength* and is distinguished from the members in *S*, which is controlled by *thrSim* (described in the lines 12 - 22 of **Algorithm 3**). Here,  $\varepsilon$  is set to 0.01 and *thrSim* is  $2*\ln(N)/N$ .

#### V. EXPERIMENTAL AND ANALYSIS

In this section, the experimental setups, including the benchmark suite, the comparison algorithms, and parameter setting are presented in Section V-A. Then, the performance measures are described in Section V-B. At last, Section V-C reports the experimental results.

#### A. Experimental Setup

To evaluate the performance of discrete MMO algorithms, we adopt the proposed benchmark suite of 25 MSTSPs, which are described in Section III. Existing discrete MMO algorithms include niching ant colony system (NACS) [20] and multi-chromosomal cramping based genetic algorithm (MCC-GA) [19]. NACS incorporates a diversity-preserving mechanism into an ant colony system to solve MSTSPs. By the diversity-preserving mechanism, multiple pheromone matrices are preserved, which guide the search of ants towards distinct directions, and thus enables the algorithm to obtain diverse solutions in parallel. MCC-GA encodes l solutions into a chromosome. The population search is devoted to finding exact l solutions. The value of lshould be given in advance. However, it is difficult to appropriately set without any prior knowledge of test instances. Therefore, as a proof of principle study, we investigate the performance of NGA and NACS on the proposed test suite.

The parameters of the NGA are empirically set: crossover rate  $P_c = 0.9$ , mutation rate  $P_m = 0.1$ , and neighborhood size m = 6. The parameters of NACS are set according to the corresponding publication [20]. The size of population is set to 150. All the algorithms terminate when the given maximum fitness evaluations (MaxFes) are exhausted. The MaxFes of 25 MSTSPs has two settings, which are listed in Table II. The algorithm should run 50 times independently to obtain the statistical results.

# B. Performance Measures

## 1) Identification of the Optimal Tours

Each of the above instances has a set of ground-truth optimal solutions, denoted as  $\mathbb{P}$ . The aim of an optimization algorithm is to locate all optima. For evaluation, we need first compare the solution set S returned by the algorithm with the ground truths to identify the optimal tours found by the algorithm by utilizing Eq. (2). A solution is considered to be optimal as long as its similarity with the one of ground-truth solutions equals to 1.

TABLE II. MAXFES APPLIED FOR 25 MSTSP INSTANCES

| MSTSP instances   | MaxFEs   |
|-------------------|----------|
| MSTSP1 - MSTSP12  | 6.00E+04 |
| MSTSP13 - MSTSP25 | 1.20E+06 |

# 1) $F_{\beta}$ Measure

Typically, an optimization algorithm will provide a final solution set S when they meet the termination condition. However, the solution set may contain many inferior and redundant solutions. To quantify the quality of the solution set, we introduce  $F_{\beta}$ , which is widely used in pattern recognition and information retrieval, as a measure.  $F_{\beta}$  is a comprehensive indicator for accessing the precision value P and the recall value R of obtained solutions. P is the fraction of the obtained solutions that are optimal solutions:

$$P = \frac{TP}{TP + FP} \tag{3}$$

where TP is the number of optimal solutions in S, and FP is the number of non-optimal solutions in S. R is the fraction of the ground-truth solutions that are successfully located:

$$R = \frac{TP}{TP + FN} \tag{4}$$

where FN is the number of optimal solutions that the algorithm misses. Actually, the sum of TP and FN is the number of total desired solutions in the benchmark.

Based on the precision and recall,  $F_{\beta}[25]$  is calculated as

$$F_{\beta} = \frac{(1+\beta^2) \cdot P \cdot R}{\beta^2 \cdot P + R} \tag{5}$$

When  $\beta$  is set to 1, it assigns the same importance to both *P* and *R*. However, for test instance with numerous optima, it is more important to locate the most representative ones than to locate all of them. So that we set  $\beta^2$  to 0.3 to magnify the effect of precision in evaluating the solutions. Besides, *P*, *R*, and  $F_{\beta}$  are real values between 0 and 1. Ideally, *P* equals to 1 when all the solutions offered by the algorithm are optimal; *R* meets 1 when all the ground-truth solutions are located by the algorithm; and subsequently,  $F_{\beta}$  achieves 1 when the values of *P* and *R* both equal to 1.

To make a further explanation, we take MSTSP9 with 4 optima as an example and compare with two different algorithms A and B. The algorithm A offers 100 solutions, whereas the algorithm B provides only 4 representative solutions. We suppose that these two algorithms successfully locate all the ground-truth solutions. It is obvious that the solution quality obtained by B is better than that obtained by A, since B provides only necessary solutions while A has redundant and inferior solutions. In the following, we give a quantitative description. For algorithm A, it has TP = 4, FP = 96, and FN = 0. Therefore, we can obtain P = 0.04 and R = 1 according to Eqs. (3) and (4). For B, it has TP = 4, FP = 0, and FN = 0 according to Eqs. (3) and (4). Therefore, we can have P = 1 and R = 1. In summary, based on Eq. (5),  $F_{\beta}$  value of A is about 0.051, while that of B is 1. From this perspective, the conclusion is consistent with the previous intuition.

#### 2) Diversity Indicator

Diversity indicator (DI) is another essential measure for evaluating the algorithm performance. When algorithms fail to locate any desired solutions, their  $F_{\beta}$  values are all zero. In these cases, the DI helps to further differentiate the performance of different algorithms. Inspired by the evolutionary multi-objective optimization area where the algorithm also provides a solution set that needs to be evaluated [22], DI measures the diversity of *S* based on the convergence of the solutions towards different optimal solutions in the ground-truth set  $\mathbb{P}$ . To be specific, DI is defined based on the average maximum similarity between the obtained solutions and the ground-truth solutions, which is calculated as

$$\mathsf{DI}(\mathcal{P},\mathcal{S}) = \frac{\sum_{i=1}^{|\mathcal{P}|} \max_{j=1,\dots,|\mathcal{S}|} \mathcal{S}(p_i, s_j)}{|\mathcal{P}|} \tag{6}$$

where  $p_i$  is the *i*th permutation of  $\mathbb{P}$ ,  $s_j$  is *j*th permutation of S, and  $S(p_i, s_j)$  is the similarity between the permutations  $p_i$  and  $s_j$  using Eq.(1).

# C. Simulation Results

The  $F_{\beta}$  and DI obtained by NACS and NGA are compared in Table III and Table IV. Better results are marked in boldface. From Table III, we find that NGA are superior to NACS on 18 out of 25 test instances in terms of  $F_{\beta}$ . However, for the last seven test instances (MSTSP19 -MSTSP25), they both get nearly zero  $F_{\beta}$  values, which indicates they fail to find any satisfactory solution in the MSTSPs with relatively large-scale cities. The observations show that the MSTSP instances with relatively large-scale cities pose a challenge to discrete MMO algorithms.

DI is presented in Table IV. The higher DI implies that the obtained solutions are more diverse. In Table IV, NGA performs better on 17 out of 25 test instances concerning DI. For the simple MSTSPs and the geometry MSTSPs, i.e., from MSTSP1 to MSTSP12, NGA is always the winner except for MSTSP5. For the composite MSTSPs (MSTSP13 - MSTSP25), NGA performs better than NACS on about half test instances, 6 out of 13. The DI values of NGA degrade along with the number of cities increasing. The observations imply that the neighborhood-based search of NGA facilitates the population diversity, but it is inadequate for relative large-scale MSTSPs.

To further investigate the significant effect with respect of  $F_{\beta}$  and DI, we also conduct the Wilcoxon rank sum test at significant level  $\alpha = 0.05$ . The results are listed in Table V. From the table, we can conclude that NGA is significantly better than NACS concerning  $F_{\beta}$  on 16 out of 25 instances, while they tie on 8 test instances. As to another indicator, DI, NGA is significantly better than NACS on 17 out of 25 instances, while NGA loses on another 8 test instances. The overall significance test results point out that the NGA outperforms in terms of both solution quality and solution diversity.

#### VI. CONCLUSION

This paper makes a preliminary study to extend the MMO into combinatorial area. To deal with combinatorial MMO problems, we incorporate a neighborhood-based strategy into GA to obtain diverse solutions. The GA facilitates global search to obtain the optimal solution, while

TABLE III.  $F_B$  of NACS and NGA

| Instance | MSTSP1  | MSTSP2  | MSTSP3  | MSTSP4  | MSTSP5  |
|----------|---------|---------|---------|---------|---------|
| NACS     | 0.684   | 0.804   | 0.497   | 0.724   | 0.989   |
| NGA      | 0.973   | 0.959   | 0.935   | 0.932   | 0.846   |
| Instance | MSTSP6  | MSTSP7  | MSTSP8  | MSTSP9  | MSTSP10 |
| NACS     | 0.643   | 0.125   | 0.137   | 0.768   | 0.813   |
| NGA      | 0.877   | 0.769   | 0.578   | 0.974   | 0.969   |
| Instance | MSTSP11 | MSTSP12 | MSTSP13 | MSTSP14 | MSTSP15 |
| NACS     | 0.459   | 0.090   | 0.025   | 0.087   | 0.004   |
| NGA      | 0.949   | 0.331   | 0.096   | 0.172   | 0.416   |
| Instance | MSTSP16 | MSTSP17 | MSTSP18 | MSTSP19 | MSTSP20 |
| NACS     | 0.000   | 0.000   | 0.000   | 0.000   | 0.000   |
| NGA      | 0.054   | 0.044   | 0.031   | 0.007   | 0.000   |
| Instance | MSTSP21 | MSTSP22 | MSTSP23 | MSTSP24 | MSTSP25 |
| NACS     | 0.012   | 0.000   | 0.000   | 0.000   | 0.000   |
| NGA      | 0.000   | 0.000   | 0.000   | 0.000   | 0.000   |

| Instance | MSTSP1  | MSTSP2  | MSTSP3  | MSTSP4  | MSTSP5  |
|----------|---------|---------|---------|---------|---------|
| NACS     | 0.788   | 0.894   | 0.757   | 0.809   | 0.983   |
| NGA      | 0.980   | 0.972   | 0.957   | 0.947   | 0.916   |
| Instance | MSTSP6  | MSTSP7  | MSTSP8  | MSTSP9  | MSTSP10 |
| NACS     | 0.843   | 0.566   | 0.652   | 0.820   | 0.850   |
| NGA      | 0.943   | 0.869   | 0.838   | 0.975   | 0.969   |
| Instance | MSTSP11 | MSTSP12 | MSTSP13 | MSTSP14 | MSTSP15 |
| NACS     | 0.758   | 0.732   | 0.752   | 0.876   | 0.744   |
| NGA      | 0.963   | 0.809   | 0.792   | 0.844   | 0.847   |
| Instance | MSTSP16 | MSTSP17 | MSTSP18 | MSTSP19 | MSTSP20 |
| NACS     | 0.680   | 0.765   | 0.671   | 0.675   | 0.745   |
| NGA      | 0.783   | 0.803   | 0.704   | 0.699   | 0.671   |
| Instance | MSTSP21 | MSTSP22 | MSTSP23 | MSTSP24 | MSTSP25 |
| NACS     | 0.773   | 0.713   | 0.671   | 0.724   | 0.725   |
| NGA      | 0.628   | 0.409   | 0.344   | 0.319   | 0.270   |
|          | •       |         |         |         |         |

TABLE V. THE SIGNIFICANT RESULTS FOR NGA AND NACS

| Wilcoxon rank sum test   | $F_{\beta}$ | DI    |
|--|-------------|-------|
| NGA vs. NACS<br>(significantly worse than/similar/significantly better than) | 1/8/16      | 8/0/1 |

the neighborhood-based strategy contributes to maintaining population diversity to locate potential candidates in parallel. Moreover, to evaluate performance of the combinatorial MMO algorithm, we propose a benchmark suite of 25 MSTSPs designed by three different methods. Furthermore, the proposed NGA and the compared NACS are utilized to solve 25 MSTSPs. We adopt two indicators to compare their performance.  $F_{\beta}$  are adospted to comprehensively assess the precision and recall values of the returned solutions, while DI measures the diversity and convergence of the obtained solutions. It is experimentally verified that NGA can achieve a competitive performance

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concerning with  $F_{\beta}$  and DI on most MSTSPs. However, they both fail to obtain any desired solutions on the MSTSP instances with large city size.

In the future work, we will improve NGA to work out the MSTSPs with large city size. In addition, we attempt to design more discrete MMO test instances to supplement the discrete benchmark.

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