

New Designs of k -means Clustering and Crossover Operator for Solving Traveling Salesman Problems using Evolutionary Algorithms

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Abstract: The traveling salesman problem is a well-known combinatorial optimization problem with permutation-based variables, which has been proven to be an NP-complete problem. Over the last few decades, many evolutionary algorithms have been developed for solving it. In this study, a new design that uses the k -means clustering method, is proposed to be used as a repairing method for the individuals in the initial population. In addition, a new crossover operator is introduced to improve the evolving process of an evolutionary algorithm and hence its performance. To investigate the performance of the proposed mechanism, two popular evolutionary algorithms (genetic algorithm and differential evolution) have been implemented for solving 18 instances of traveling salesman problems and the results have been compared with those obtained from standard versions of GA and DE, and 3 other state-of-the-art algorithms. Results show that the proposed components can significantly improve the performance of EAs while solving TSPs with small, medium and large-sized problems.

1 INTRODUCTION

The traveling salesman problem (TSP) is a prevalent mathematics problem that requests the shortest possible distance to visit a set of cities. Despite the simplicity of its definition, TSP is one of the most challenging combinatorial optimization problems (COPs) in real world. Its practical importance is shown in many fields, such as operational research, algorithms design and artificial intelligence, and also in many engineering applications, like design of hardware devices and radio electronic systems, and computer networks (Evans, 2017). So, it attracted the attention of several researches for many years to find the best way for optimally solving TSPs in a reasonable computational time.

Many exact algorithms, which can accurately find the optimum solution, have been introduced for solving TSPs (Miller and Pekny, 1991). However, they have been considered inapplicable for solving many instances of TSPs, which were proven to be an NP-hard COP (Jünger et al., 1995). In recent years,

several heuristics methods, which can find near optimum solution, have been developed for TSPs and they achieved better results than exact ones in terms of computational time. Among these methods, evolutionary algorithms (EAs), which demonstrate a very promising direction for TSPs. EAs are inspired by the biological model of evolution and natural selection, and they have a long history of successfully solving optimization problems (Bäck et al., 2018).

Many EAs-based approaches have been introduced for solving TSPs. Some of them were integrating local searches (Mavrovouniotis et al., 2017), and these studies showed that incorporation of local search operators can significantly improve the performance of EAs. Other EAs, such as genetic algorithms (GAs) and differential evolution (DE) algorithms have also been developed for TSPs. Recently, GA, with two local operators, called branch and bound, and cross elimination, was used for solving multiple TSPs (Lo et al., 2018). A new initial population strategy, based on k -means algorithm, was also proposed to improve the performance of GA

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(Deng et al., 2015). Although the algorithm achieved better error values than the random generation, the obtained error values are still away from the optimal solutions. Moreover, many DE algorithms have been introduced for TSPs (Wei et al., 2016, Wang and Xu, 2011). However, many of the studies have been tested on small and medium TSPs.

Seeking to improve the performance of EAs and overcome some limitations that presented in the previous research works, such as slow convergence, increased computational time, and poor quality of solutions, the following contributions are proposed in this paper: 1) a new design of k -means clustering to be used as a repairing method for the generated individuals in the initial population, which can increase the convergence speed of an EA and increase the possibility of getting the optimal solution in a lower computational time; 2) a new crossover operator, which is designed based on the characteristics of TSPs to increase the population diversity and improve the evolving processes of an EAs. Finally, the proposed components have been implemented using GA and DE for solving different instances of TSP and the results were compared with those from state-of-the-art algorithms and standard versions of GA and DE.

The rest of this paper is organized as follows. Section 2 presents the objective function of TSPs and the original structures of GA and DE. Section 3 represents the proposed components. Section 4 discusses the experimental results and comparisons. Finally, conclusion drawn from this study and future work are provided in Section 5.

2 BACKGROUND

In this section, the definition and objective function of TSPs, and the standard versions of GA and DE are introduced.

2.1 Traveling Salesman Problem

The traveling salesman problem (TSP) is a well-known COP with discrete decision variables. In 1930, TSP was formulated as a mathematical problem for the first time. In traditional TSP, a person has a task of visiting N numbers of cities. He needs to visit every city only once in any order starting from any city and returning back to the home city from where he started. Given the distances between each city, the person needs to minimize the total travelled distance during his trip. The objective is to find the shortest tour that visits each city exactly ones, and then return

to the starting city. Mathematically, the objective function of TSP can be described as minimization of the total distances between visited cities, in addition to the distance of returning to start city, as follows:

Minimize: D , where

$$D = d_{N,1} + \sum_{i=1}^{N-1} d_{i,i+1} \quad (1)$$

where D is the total distance of the trip, N is the number of cities to be visited, $i = 1, 2, \dots, N$. $d_{N,1}$ is the return distance from the last city (N) to the first one, and $d_{i,i+1}$ is the distance between two consecutive cities i and $i + 1$.

2.2 Standard Versions of Genetic Algorithm and Differential Evolution

Both GA and DE belong to EAs (Bäck et al., 2018). They solve a problem by iteratively improving the candidate solutions through three evolving operators, namely: mutation, crossover and selection. These operators are applied to guide the search to find optimal solutions. The first basic difference between GA and DE is the order of evolving operators' execution, as GA applies selection then crossover and finally mutation, whereas DE considers mutation first, then crossover and selection. The second major difference is that GA performs an additional process called elitism, which ensures that the best individual from the current generation is carried over to the next without any modifications. This process guarantees that the quality of the solutions is not decreased from one generation to another. GA and DE are considered powerful tools for solving optimization problems in both continuous and discrete spaces. Basically, an initial population with a pre-determined size (PS) is generated and then each individual (\vec{x}_i), which consists of N variables, is evolved using the three evolutionary operators. Figure 1 shows the basic outlines of the standard versions of GA and DE and the order of their three evolving operators.

2.2.1 Mutation Operator

In DE, a mutant vector is generated for each target vector ($x_{i,g}$), using this simplest mutation form:

$$\vec{v}_{i,g+1} = \vec{x}_{r_1,g} + F \times (\vec{x}_{r_2,g} - \vec{x}_{r_3,g}), \quad r_1 \neq r_2 \neq r_3 \neq i \quad (2)$$

where F is the weighting factor, that controls the amplification of the differential variation between the

two vectors $\vec{x}_{r_2,g}$ and $\vec{x}_{r_3,g}$, and generally lies within the range of $[0, 2]$. $\vec{x}_{r_1,g}$, $\vec{x}_{r_2,g}$, $\vec{x}_{r_3,g}$ are three randomly chosen vectors, which are not equal to each other or to the target vector ($\vec{x}_{i,g}$). In GA, mutation modifies one or more gene values in an individual by swapping them with other genes or flip their values from the initial state, and hence the individual may change entirely from the previous one.

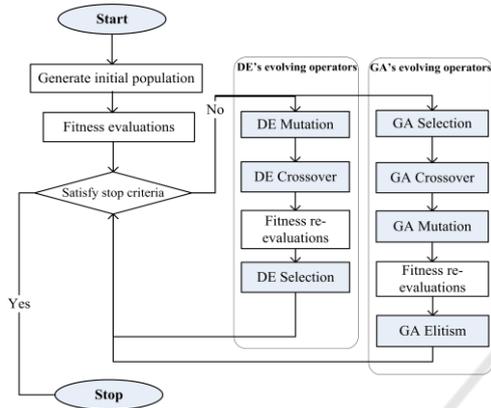


Figure 1: Structure of standard GA and DE.

2.2.2 Crossover Operator

In DE, new vectors (trial vectors) are generated by combining target (individuals from last generation) and mutant vectors according to a pre-defined possibility. Binomial and exponential are the two most well-known types of crossover for DE. In GA, the new offspring is produced by exchanging different parts of two randomly selected parents, where if the first part of the offspring came from first parent, the second part must come from second parent, etc. This is called one-point crossover (Ali et al., 2015), where a random point is generated to divide both parents into two parts.

2.2.3 Selection Operator

In DE, a comparison of each trial vector and its corresponding target vector is used to determine whether trail or target vectors should survive to the next generation. The greedy strategy is an example of DE selection operator. In GA, a tournament method is adopted to select an individual by running several competitions, based on the fitness values and the feasibility of the solutions, among a few individuals selected randomly from the population.

In both GA and DE, the processes of the evolutionary operations remain as long as a time or a generation limit is reached, or the number of calling

the fitness evaluation function is greater than a pre-defined number of calling.

3 PROPOSED EVOLUTIONARY ALGORITHM

In this paper, two main components have been developed and implemented in order to improve the performance of EAs for solving TSPs. In this section, the basic steps of EAs and the two proposed components are briefly discussed. Figure 2 shows the proposed components when adopting with both GA and DE algorithms as examples of EAs.

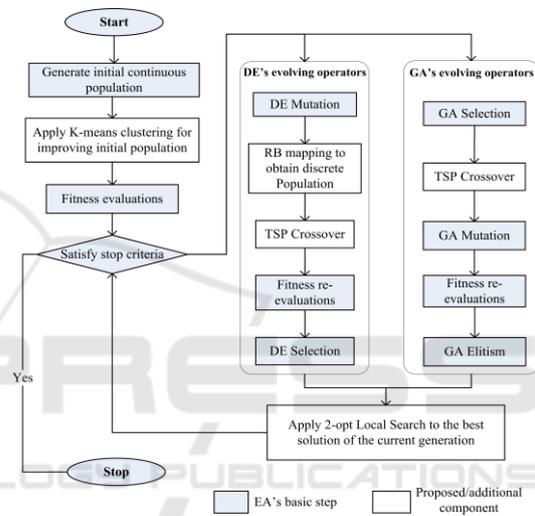


Figure 2: Structure of proposed GA and DE.

3.1 Initial Population

The first step in most EA is to generate an initial population of solutions. So, a population of PS solutions is randomly generated. In our algorithm, every solution can be represented by a discrete vector, where the length of each vector equals the number of cities to be visited (N).

3.2 k-means Clustering as a Repairing Method

As TSPs are a complex COP, we noticed that the evolutionary process may take longer to make the solutions in the initial population converge towards the optimal solution. So, a new design of k -means clustering method is applied, according to a pre-defined probability ($ClusProb$), to the solutions in the initial population as a repairing method to

improve their qualities within the initial phase, and as a result, the optimal solution is likely to be found after a few EA's generations.

In k -means clustering, several locations (L) are generated over the geometric problem space according to Equation 3. A number of groups, equal to L , are formed with those points as the centroids. Each group attracts the close cities (by their coordinates) from its centroid.

$$L = \text{round}(\sqrt{N} + 0.5) \quad (3)$$

After assigning all the cities in groups, each group is solved as a sub-TSP by finding the shortest sub-tour between the cities in each group. In order to form the complete tour of TSP, the distances between the centroid points (L) are calculated and the two groups with the smallest distance between their centroids are selected to be merged and form a larger group. The merge between groups is done by connecting two cities of a group with their closest two cities of the other group after breaking their local connections. After that, the centroid point of the new formed group is calculated and the distances between all the centroid points ($L - 1$) of existing groups are remeasured. This process is repeated until only one group ($L = 1$) that contains all the cities is formed.

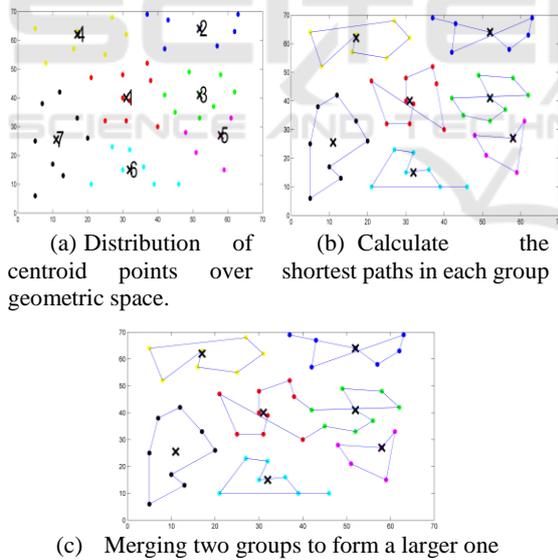


Figure 3: Steps of k -means clustering repairing method.

In Figure 3, the basic steps of k -means clustering repairing method are illustrated. It shows the steps of the proposed repairing method, for a TSP instance called *eil51* with 51 cities to be visited, as follows: (a) gives the distribution of the L locations over the search space of the problem; (b) shows the shortest path in each formed group; (c) displays the generation

of the first group produced from merging group 1 with 3. This last step is repeated until one large group including all the cities is formed with the shortest path between them, as the example shown in Figure 4.

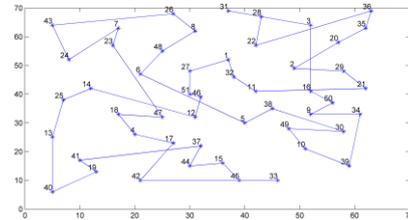


Figure 4: Final tour after applying k -means clustering repairing method.

3.3 Fitness Evaluations

After the initial population is generated and repaired, the fitness value of each individual is measured seeking to rank them according to their qualities. The fitness function shown on Equation 1 is used to calculate the quality of each solution, and then the solutions are ranked where the fittest one shown first and the worst last.

3.4 Evolving Operators

3.4.1 Proposed Crossover for TSP

In this paper, a new design of a crossover, which uses the characteristics of the TSP (TSP-Xover) is given. In TSP-Xover, the one-point crossover procedure is followed, where a random cut point (CP) in the range $[1, N]$ is chosen and two parents are randomly selected to generate a new offspring. The first part of the offspring $[1, 2, \dots, CP]$ is copied from one of the parents, and the second part is completed from the other. In order to do that, starting from the last city in the first part of the offspring (CP), the next city ($CP + 1$) is selected based on its distance from CP . So, if the next city is the closest one to the CP city and has not been taken before in the offspring (not in the range $[1 - CP]$), then next city will be added in offspring at ($CP + 1$) order. The pseudo-code for the proposed crossover (TSP-Xover) is provided in Algorithm 1.

3.4.2 Mutation Operator

The standard mutation operators of GA and DE were implemented in the proposed framework. For DE and GA, the $DE/rand/1$ mutation strategy (Equation 2) and the swap mutation (Bäck et al., 2018) were adopted, respectively.

Algorithm 1: Pseudo-code of TSP-Xover.

```

for  $i$  form 1 to  $PS$  do
  if random-number  $\leq cr$  then
    Parent1  $\leftarrow$  random individual
    Parent2  $\leftarrow$  another random individual
     $CP \leftarrow$  random point in range  $[1 - N]$ 
     $Dis \leftarrow$  Distance between all cities
    Offspring=Parent1(1 to  $CP$ )
     $j \leftarrow CP + 1$ 
    while  $j \leq N$  do
      SelectedCity  $\leftarrow$  city from Parent2
      with  $\min(Dis(Parent1(j-1)$  and
      Parent2(1 to  $N)))$ 
      if SelectedCity is not existed in
      Offspring(1 to  $j-1$ ), then
        Offspring( $j$ )  $\leftarrow$  SelectedCity
         $j \leftarrow j + 1$ 
      else
        SelectedCity  $\leftarrow$  next closest city
        from Parent2
      end if
    end while
  end if
end for

```

3.5 Fitness Re-evaluations and Selection

After obtaining the new population, a selection operator is applied to decide which solution can survive to the next generation. The greedy selection strategy and the tournament method are applied to DE and GA, respectively. The solutions in the new selected population are ranked based on their fitness values, where the best solution located first.

For comparisons purposes, 2-Opt local search (Savelsbergh, 1985) is used and applied to the best solution found in each generation for all standard and proposed versions of GA and DE.

3.6 Termination Condition

In this study, the number of calling the fitness function is counted and if this counter exceeds the predefined allowed number of objective function evaluations, the algorithm is terminated.

4 EXPERIMENTAL RESULTS

To judge the effect of the proposed components on the performance of EAs, computational simulations were carried out using GA and DE (as popular examples of EAs) for solving 18 instances of TSPs

with small, medium and large dimensions. The instances were selected from the well-known TSP library (TSPLIB), which is described in (Reinelt, 1991). Both GA and DE were coded in MATLAB R2017b, and were performed on a PC with an i7 Processor and 16 GB memory. In our experiments, each TSP instance was independently executed 30 times with 1,000, 5,000 and 50,000 fitness evaluations in each run for comparison. The quality of each algorithm is assessed by calculating the average error of each problem, which is the error between the best obtained solution by an algorithm and the optimal solution of the same problem as shown in Equation 4.

$$Average\ error = \left(\frac{Best - Optimal}{Best} \right) \times 100 \quad (4)$$

4.1 Parameters Settings and Tuning

In this sub-section, the parameters setup of both GA and DE and the parameter analyses of the two proposed components are presented.

4.1.1 Parameter Settings

Based on extensive experiments using 18 instances of TSPs, the final parameters setup of GA and DE are shown in Table 1.

Table 1: GA and DE parameters setup.

Parameter	Symbol	Value
Number of runs		30
Population size	PS	50
Crossover rate	cr	0.7
Mutation rate	F	0.2
Number of individuals to be repaired in the initial population	$ClusProb$	0.1 (10%)
Maximum fitness evaluations		1000, 5000, and 50,000

4.1.2 Parameters Tuning

Two sets of experiments were designed to analyse effects of the two proposed components' parameters $ClusProb$ and cr , while the other parameters' values were fixed as shown in Table I. Both $ClusProb$, and cr , were run with different values for 10 runs for each value and 5000 fitness evaluations for each run using GA and DE for solving 18 TSPs. Figures 5 and 6 present the average value of errors of solved TSPs from their optimal solutions (on bars) and standard deviations (on vertical small bars) using DE and GA, respectively. In the figures, DE and GA run with $ClusProb$ set to different values of 0, 10, 30, 50, 70, 90 and 100 (%) of PS . The results show that repairing

10% of the individuals in the initial population can enhance the average error by 47.98% and 61.21% compared with the average of other parameter values in DE and GA, respectively. Also, we noticed that with higher values of *ClusProb*, the average error is increased because of the lack of diversity in the population. On the other hand, *ClusProb* =0%, achieved worse average error than *ClusProb*=10%, which confirms the importance of the proposed repairing method. Another experiment run for analysing *cr* parameter by setting it to different values of 0.1, 0.3, 0.5, 0.7 and 0.9. Based on the results, it was found that *cr*=0.7 achieved the best average error compared with other values.

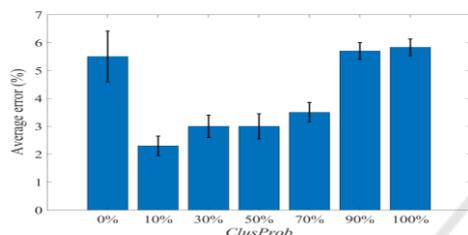


Figure 5: Analysis of *ClusProb* parameter with standard deviation error bar using DE.

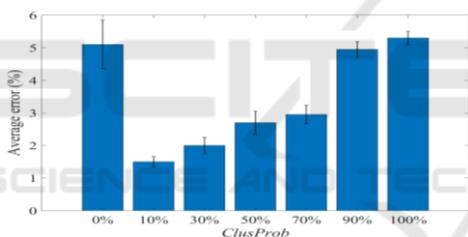


Figure 6: Analysis of *ClusProb* parameter with standard deviation error bar using GA.

4.2 Effect of *k*-means Clustering Repairing Method

This sub-section discusses the effect of applying the proposed repairing method on performance of an EA. In order to do that, all TSPs have been solved with and without applying *k*-means method. Results show that the proposed method can enhance the quality of solutions by 76.6% on average. To graphically present the effect of the proposed method, the best individuals of 3 TSPs were presented before and after adopting the proposed method in Figure 7.

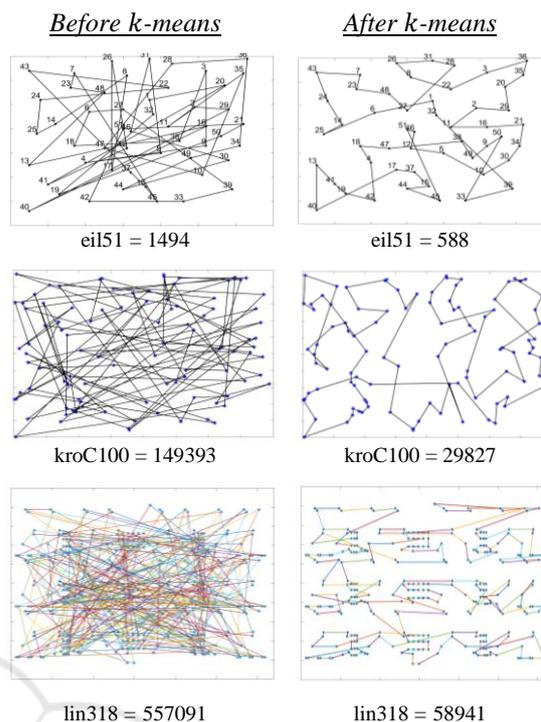


Figure 7: Graphical paths of 3 TSPs before and after applying the proposed repairing method with the total distance of each.

For comparison, Figure 7 shows the paths of the same individual of each problem produced directly after generation of the initial population (*Before k-means*) and after being repaired (*After k-means*). The figure also provides the total distances of each individual to show differences in their qualities. From Figure 7, it can be noticed that *k*-means clustering repairing method can enhance the solutions in the initial population for TSPs “eil51”, “kroC100”, and “lin318” by 60.64%, 80%, 89.41%, respectively. The results demonstrate efficiency of the proposed repairing method, especially for large TSP instances.

4.3 Comparison with Standard Versions of GA and DE

In order to judge the effect of the proposed components on the overall performance of EAs, in this sub-section the performances of GA and DE will be compared, with and without, incorporating the proposed components. In order to do that, the best and mean values of the average errors produced from i) standard GA, ii) standard DE, iii) GA + *k*-means and TSP-Xover, and iv) DE + *k*-means and TSP-Xover are presented in Table 2.

Table 2: Best (B) and mean (M) average errors for 18 instances of TSPs obtained from improved and standard versions of GA and DE.

Probs	Standard GA		GA + k - means and TSP-Xover		Standard DE		DE + k - means and TSP-Xover	
	B	M	B	M	B	M	B	M
eil51	0.0	2.0	0.0	0.8	0.5	1.7	0.2	1.2
berlin52	0.3	2.0	0.0	0.1	0.0	2.2	0.0	0.6
st70	0.2	2.7	0.0	0.6	1.2	2.0	0.3	1.5
eil76	0.2	2.7	0.7	2.5	2.0	4.0	1.9	3.6
pr76	1.6	2.0	0.0	0.5	0.0	1.3	0.0	1.2
kroA100	0.2	1.0	0.0	3.9	0.8	1.9	0.8	2.1
kroC100	0.5	1.7	0.0	3.9	1.0	2.8	1.0	2.7
kroD100	1.1	2.4	0.0	3.9	1.8	3.2	1.6	3.2
eil101	2.7	4.1	0.0	2.5	3.3	5.2	3.0	5.3
lin105	0.4	4.0	0.0	1.0	0.6	1.8	0.2	1.5
pr144	0.1	1.7	0.1	0.5	0.1	0.4	0.1	0.5
ch150	2.9	4.6	0.0	5.1	3.2	4.8	2.8	4.7
kroA150	2.0	4.0	0.1	5.1	2.5	4.2	1.3	4.3
kroB150	2.1	3.6	1.0	5.5	2.3	3.8	2.0	3.9
pr152	0.5	2.1	0.2	3.6	1.2	2.2	1.1	2.3
lin318	4.0	5.7	0.9	7.0	3.8	5.5	3.9	5.5
pcb442	5.8	7.5	0.1	8.1	6.2	7.9	6.0	7.6
d493	4.5	6.3	0.8	7.2	5.2	6.2	5.0	6.3
Avg.	1.6	3.3	0.2	3.4	2.0	3.4	1.7	3.2

A nonparametric statistical test (Woolson, 2007), which is usually used to assess whether the population mean ranks of two related samples differ, is applied to show the significant differences between the proposed versions of GA and DE and their standard versions. The outcome is listed in Table 3.

Table 3: Nonparametric Wilcoxon test based on the best and mean errors from the optimal solution.

		Better	Equal	Worse	P.Value
GA + k-means and TSP-Xover VS. Standard GA	Best	15	1	2	0.001
	Mean	10	0	8	0.931
DE + k-means and TSP-Xover VS. Standard DE	Best	14	2	2	0.002
	Mean	10	0	8	0.338

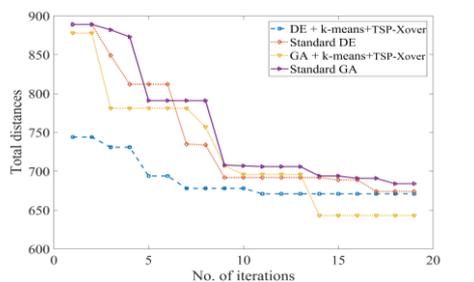


Figure 8: Convergence plot of *eil101* TSP with 20 iterations (1000 fitness evaluations).

From results in Table 2 and 3, the versions with the added proposed components can significantly enhance the performances of the standard GA and DE by 86.52% and 12.13% in terms of the best errors from the optimal solutions of 18 TSPs.

To graphically represent the performance of each algorithm, the convergence plot of one TSP, namely: *eil101* is shown in Figure 8.

4.4 Comparison with State-of-the-Art Algorithms

In this sub-section, the performance of the proposed algorithm is compared with three algorithms from the state-of-the-art algorithms: 1) improved bat algorithm (IBA) (Osaba et al., 2016); 2) Discrete firefly algorithm (DFA) (Osaba et al., 2016); and 3) a discrete imperialist competitive algorithm (DICA) (Osaba et al., 2016), as shown in Table 4.

Table 4: Total distances obtained from the proposed versions of GA and DE and 3 state-of-the-art algorithms.

Probs	GA + k - means and TSP-Xover	DE + k - means and TSP-Xover	IBA	DFA	DICA
eil51	426	427	426	426	426
berlin52	7542	7542	7542	7542	7542
st70	675	676	675	675	675
eil76	539	540	539	543	544

Table 4 shows the competitive performance of the proposed components with GA and DE compared with other evolutionary algorithms. However, the results didn't show any differences between the comparative algorithms.

In order to further assess the performance of the proposed components, the proposed GA is compared with other three algorithms: 1) GA, 2) PSO, and 3) hybrid GA-PSO, which were recently proposed in (Gupta et al., 2019).

Table 5: Average error % (E) and average time in seconds (T) obtained from the proposed GA and other 3 algorithms.

Probs.	GA		PSO		GA-PSO		Proposed GA	
	E	T	E	T	E	T	E	T
ATT48	2.4	0.5	2.8	0.4	0.3	0.4	0.5	0.5
EIL51	2.6	0.6	3.1	0.4	1.2	0.5	1.2	0.5
ST70	4.2	0.9	4.9	0.6	0.8	0.7	0.1	0.7
PR76	2.2	1.2	2.6	0.8	0.7	1.0	0.4	1.6
RD100	4.5	1.8	5.3	1.3	1.6	1.5	0.0	1.5
KROA100	4.0	1.8	4.8	1.3	1.0	1.5	0.1	1.5
KROB100	3.1	1.8	3.7	1.2	1.8	1.5	0.1	1.3
PR107	3.2	2.1	3.8	1.5	1.2	1.7	0.0	1.8
PR124	2.0	2.4	2.4	1.6	0.3	2.1	0.0	2.3
GIL262	6.3	10.0	7.5	7.1	3.0	8.6	0.0	7.3
Average	3.4	2.3	4.1	1.6	1.2	2.0	0.3	1.9

Table 5 showed that the GA version with the proposed components can achieve a higher average error from the optimal solution than other comparative algorithms for the first three (small) TSPs. However, starting from the fourth problem, the proposed GA achieved the best average error compared with others. This indicates that the proposed components are more suitable to solve TSPs with large sizes. The average values showed that the proposed GA can achieve better average errors by 92.55%, 93.70%, and 78.18% than GA, PSO, and hybrid GA-PSO, respectively.

Moreover, the detailed results of the proposed GA and other comparative algorithms are shown in Table 1 in the Appendix, which can be accessed from <https://github.com/IsmailMALi/TSP-Results>. In Table 1, the results of 10 TSPs with different number of cities, mean values, average error (%), and average computational time in seconds, are given.

5 CONCLUSION AND FUTURE WORK

In this paper, a new design that uses the k -means clustering as a repairing method for the initial population of an EA, and a new crossover strategy for TSPs, are proposed. The k -means clustering repairing method is applied directly after the initial population is generated to enhance the quality of the solutions. The crossover is designed to generate offspring from the current individuals taking in account the characteristics of the TSP. The experimental results showed that these proposed components can significantly improve the performance of EAs, while solving TSPs and are very promising especially when dealing with large TSPs.

In the future, more complex discrete problems, such as resource constrained project scheduling problems (RCPSPs) and traveling thief problems (TTPs), will be used to test the effectiveness of the proposed components while solving such problems.

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