# Solving the Clustered Traveling Salesman Problem via TSP methods

Yongliang Lu<sup>a</sup>, Jin-Kao Hao<sup>b</sup>, Qinghua Wu<sup>c,\*</sup>,

<sup>a</sup>School of Economics and Management, Fuzhou University, 350116 Fuzhou, China

<sup>b</sup>LERIA, Université d'Angers, 2 Boulevard Lavoisier, 49045 Angers, France <sup>c</sup>School of Management, Huazhong University of Science and Technology, Wuhan, China, email: qinghuawu1005@gmail.com

To appear in PeerJ Computer Science, April 2022

#### Abstract

The Clustered Traveling Salesman Problem (CTSP) is a variant of the popular Traveling Salesman Problem (TSP) arising from a number of real-life applications. In this work, we explore a transformation approach that solves the CTSP by converting it to the well-studied TSP. For this purpose, we first investigate a technique to convert a CTSP instance to a TSP and then apply powerful TSP solvers (including exact and heuristic solvers) to solve the resulting TSP instance. We want to answer the following questions: How do state-of-the-art TSP solvers perform on clustered instances converted from the CTSP? Do state-of-the-art TSP solvers compete well with the best performing methods specifically designed for the CTSP? For this purpose, we present intensive computational experiments on various benchmark instances to draw conclusions.

Keywords: Traveling salesman; Heuristics; Clustered traveling salesman; Problem transformation

# 1 Introduction

The Clustered Traveling Salesman Problem (CTSP), originally proposed by Chisman (1975), is an extension of the classic Traveling Salesman Problem (TSP) where the cities are grouped into clusters and the cities of each cluster must be visited contiguously. Formally, the problem is defined on a symmetric complete weighted graph G = (V, E) with a set of vertices  $V = \{1, 2, ..., n\}$ 

<sup>\*</sup> Corresponding author.

and a set of edges  $E = \{(i, j) : i, j \in V, i \neq j\}$ . The vertex set V is partitioned into disjoint clusters  $V_1, V_2, ..., V_m$  ( $V_1 \cup V_2 \cup ... \cup V_m = V$ ). Let C be an  $n \times n$  symmetric distance matrix such that  $c_{ij}$  ( $i, j = 1, 2..., n, i \neq j$ ) represents the travel cost between two corresponding vertices i and j, and satisfies the triangle inequality rule. The objective of the CTSP is to find a minimum cost Hamiltonian circuit over all the vertices, where the vertices of each cluster must be visited consecutively.

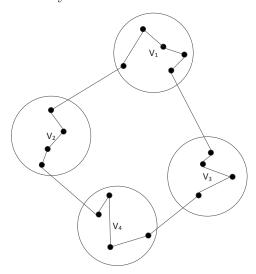


Fig. 1. A feasible solution for an instance of the CTSP

Fig. 1 shows a feasible solution for a CTSP instance, where the solution corresponds to a Hamiltonian cycle such that the vertices of each cluster are visited contiguously.

The CTSP can be formally modelled as the following integer programming model described in Chisman (1975), where without loss of generality, the salesman is assumed to leave origin city 1 and return to 1.

$$\min f = \sum_{i=1}^{n} \sum_{j=1}^{n} c_{ij} x_{ij} \tag{1}$$

subject to

$$\sum_{j=1}^{n} x_{ij} = 1 \qquad \forall i \in V \tag{2}$$

$$\sum_{i=1}^{n} x_{ij} = 1 \qquad \forall j \in V \tag{3}$$

$$u_i - u_j + (n-1)x_{ij} \le n-2$$
  $2 \le i \ne j \le n$  (4)

$$\sum_{i \in V_k} \sum_{j \in V_k} x_{ij} = |V_k| - 1 \qquad \forall V_k \subset V, |V_k| \ge 1, k = 1, 2, ..., m$$
 (5)

$$x_{ij} \in \{0, 1\} \qquad \forall i, j \in V \tag{6}$$

$$u_i \ge 0 \qquad 2 \le i \le n \tag{7}$$

In this model, the binary variable  $x_{ij} = 1$  if city j is visited immediately after city i;  $x_{ij} = 0$  otherwise. Objective function (1) seeks to minimize the total distance traveled by the salesman. Constraints (2) and (3) ensure that each city is visited exactly once. Constraints (4) eliminate subtours, while constraints (5) guarantee that the cities of each cluster are visited contiguously. The remaining constraints are related to the decision variables.

The above subtour elimination constraints (4) are called MTZ formulation (Miller et al., 1960). Although MTZ is simple to implement, it provides a very poor linear relaxation (Campuzano et al., 2020). Many compact formulations have been proposed to replace Constraints (4). According to the literature, a multi-commodity flow formulation (Wong, 1980; Claus, 1984) was proven to provide a strong linear relaxation, without compromising its simplicity. In the multi-commodity flow formulation, let k = 2, 3, ..., n be n - 1 commodities, and let  $y_{ij}^k$  be a nonnegative decision variable which represents the flow on the arc  $(i, j) \in E$  for the commodity k from city 1 to city k. Then, another alternative mathematical model for the CTSP is constituted of the objective function (1) and the constraints (2), (3), (5), (6) along with the following subtour elimination constraints:

$$0 \le y_{ij}^k \le x_{ij} \qquad \forall i, j, k \in V, k \ne 1 \tag{8}$$

$$\sum_{i=2}^{n} y_{1i}^{k} = 1 \qquad \forall k \in V \setminus \{1\}$$
 (9)

$$\sum_{i=2}^{n} y_{i1}^{k} = 0 \qquad \forall k \in V \setminus \{1\}$$
 (10)

$$\sum_{i=1}^{n} y_{ik}^{k} = 1 \qquad \forall k \in V \setminus \{1\}$$
 (11)

$$\sum_{j=1}^{n} y_{kj}^{k} = 0 \qquad \forall k \in V \setminus \{1\}$$
 (12)

$$\sum_{i=1}^{n} y_{ij}^{k} - \sum_{i=1}^{n} y_{ji}^{k} = 0 \qquad \forall j, k \in V \setminus \{1\}, j \neq k$$
 (13)

Constraints (8) only allow flow in an arc (i, j) if and only if it is traversed by the salesman (i.e.,  $x_{ij} = 1$ ). Constraints (9) ensure that city 1 is the source of one unit of each commodity  $k \in V \setminus \{1\}$  and Constraints (10) avoid that the flow of each commodity  $k \in V \setminus \{1\}$  returns to city 1. Constraints (11) and (12) guarantees that one flow unit of commodity k enters to city k and

it does not leave the city k. Constraints (13) ensure flow conservation at each city, apart from city 1 and for commodity k at city k.

One notices that the CTSP is equivalent to the TSP when there is a single cluster or when each cluster contains exactly one vertex. Therefore, the CTSP is NP-hard, and thus computationally challenging in the general case. From a practical perspective, the CTSP is a versatile modeling tool for several operational research applications arising in a wide variety of areas, including automated warehouse routing (Chisman, 1975), emergency vehicle dispatching (Weintraub et al., 1999), production planning (Lokin, 1979), disk defragmentation (Laporte and Palekar, 2002), and commercial transactions with supermarkets, shops and grocery suppliers (Ghaziri and Osman, 2003). As a result, effective solution methods for the CTSP can help to solve these practical problems. Indeed, the computational challenge and the wide range of applications of the problem have motivated a variety of approaches that are reviewed in Section 2. However, unlike the classic TSP problem for which many powerful methods have been introduced in the past decades, studies on the CTSP are still quite limited.

Moreover, the CTSP belongs to the large class of traveling salesman problems. Among the TSP variants, the generalized traveling salesman problem (GTSP) (Srivastava et al., 1969; Cosma et al., 2021) and the family traveling salesman problem (FTSP) (Morán-Mirabal et al., 2014; Pop et al., 2018) share similarities with the CTSP. In the GTSP, the set of vertices is divided into clusters and the objective is to find a minimum-cost tour passing through one vertex from each cluster. In the FTSP, the set of vertices is also divided into clusters (called families) and the objective is to visit a predefined number of vertices in each family at a minimum cost.

In this work, we investigate the problem transformation approach proposed in Chisman (1975), which converts the CTSP to the TSP and assess the interest of popular modern TSP solvers for solving the resulting TSP instances. To our knowledge, this is the first large computational study testing modern TSP solvers on solving the CTSP. The work is motivated by the following considerations. First, intensive researches on the TSP have led to the development of many very powerful solvers. Thus, it is interesting to know whether we can take advantage of these solvers to effectively solve the CTSP. Second, the TSP instances converted from the CTSP are characterized by their cluster structures. These instances constitute interesting test cases for existing TSP solvers. This work aims thus to answer the following questions.

- 1. How do state-of-the-art *exact* TSP solvers perform on clustered instances converted from the CTSP?
- 2. How do state-of-the-art *inexact* (heuristic) TSP solvers perform on clustered instances converted from the CTSP?

3. Do state-of-the-art TSP solvers compete well with the best performing methods specifically designed for the CTSP?

To our knowledge, Questions 1 and 3 have never been investigated in the literature. Regarding Question 2, two previous studies (Neto, 1999; Helsgaun, 2014) are of interest. However, they are limited because they only concern one TSP algorithm, i.e., the local search based LKH solver (Helsgaun, 2009), while ignoring other powerful TSP solvers like GA-EAX (Nagata and Kobayashi, 1997) and Concorde (Applegate et al., 2006a). Answering these questions helps to enrich the state-of-the-art of solving the CTSP and gain novel knowledge on using modern TSP methods to solve new problems. Finally, we mention that the transformation approach was also tested in Lokin (1979) and Jongens and Volgenant (1985). However, these studies are clearly outdated and don't provide useful information as to the questions we want to investigate.

The remainder of this paper is organized as follows. Section 2 reviews existing solution methods for the CTSP. Section 3 presents the transformation of the CTSP to the TSP and three powerful TSP methods (solvers). Section 4 shows computational studies of the TSP solvers applied to the clustered instances and comparisons with existing algorithms dedicated to the CTSP. Section 5 provides additional explanations regarding the behaviors of the three TSP solvers. Finally, concluding remarks are provided in Section 6.

#### 2 Literature review on existing solution methods

There are several dedicated solution algorithms for solving the CTSP that are based on exact, approximation, and metaheuristic approaches.

Along with the introduction of the CTSP, Chisman (1975) proposed a branchand-bound algorithm to solve the integer programming model presented in the Introduction section. Jongens and Volgenant (1985) developed an algorithm based on the 1-tree relaxation to provide lower bounds as well as a heuristic to find satisfactory upper bounds. Mestria et al. (2013) used the mathematical formulation of Chisman (1975) and IBM Parallel CPLEX solver (version 11.2) to obtain lower bounds for medium CTSP instances ( $|V| \leq 1000$ ).

Various a-approximation algorithms (Anily et al., 1999; Gendreau et al., 1997; Guttmann-Beck et al., 2000) have been developed for the CTSP. These approximation algorithms require either the starting and ending vertices in each cluster or a prespecified order of visiting the clusters in the tour as inputs, and solve the inter-cluster and intra-cluster problems independently. Bao and Liu (2012) presented a new 2.17-approximation algorithm where no starting and ending vertices were specified. Later, Bao et al. (2017) provided a 2.5-

approximation algorithm for another version of the CTSP where the starting vertex of each cluster is given while the ending vertex is not specified. Recently, Kawasaki and Takazawa (2020) improved the approximation ratio for the CTSP by incorporating a recent approximation algorithm for the TSP by Zenklusen (2019).

Given that the CTSP is a NP-hard problem, a number of heuristic and metaheuristic algorithms have also been investigated, which aim to provide high-quality solutions in acceptable computation time, but without provable optimal guarantee of the attained solutions. For example, Laporte et al. (1997) presented a tabu search algorithm to solve a particular case of the CTSP, where the clusters are visited in a prespecified order. Potvin and Guertin (1996) developed a genetic algorithm for the CTSP that finds inter-cluster paths and then intra-cluster paths. Later, Ding et al. (2007) proposed a two-level genetic algorithm for the CTSP. In the first level, a genetic algorithm is used to find the shortest Hamiltonian cycle for each cluster. In the second level, a modified genetic algorithm is applied to merge the Hamiltonian cycles of all the clusters into a complete tour.

In addition to these early heuristic algorithms, Mestria et al. (2013) investigated GRASP (Greedy Randomized Adaptive Search Procedure) with pathrelinking. Among the six proposed heuristics, one heuristic corresponds to the traditional GRASP procedure whereas the other heuristics include different path relinking procedures. Mestria (2016) studied a hybrid heuristic, which is based on a combination of GRASP, Iterated Local Search (ILS) and Variable Neighborhood Descent (VND). Recently, Mestria (2018) presented another complex hybrid algorithm (VNRDGILS) which mixes GRASP, ILS, and Variable Neighborhood Random Descent to explore several neighborhoods. According to the computational results reported in Mestria et al. (2013); Mestria (2016, 2018), these GRASP-based algorithms are among the best performing heuristics specially designed for the CTSP currently available in the literature. In addition, Hà et al. (2022) proposed a metaheuristic method based on the ILS framework with problem-tailored operators for a version of the CTSP where the order of visiting the clusters is prespecified.

Existing studies have significantly contributed to better solving the CTSP. According to the computational results reported in the literature, due to the NP-hardness of the problem, only small CTSP instances were able to be solved to optimality with the exact algorithms. The approximation algorithms provide solutions for the CTSP within a given approximation factor. However, due to the high approximation factors involved (e.g., 5/3 (Anily et al., 1999), 3/2 Gendreau et al. (1997), 2.17 (Bao and Liu, 2012), and 2.5 (Bao et al., 2017)), these approximation algorithms are not practical for solving large instances. To deal with large CTSP instances, heuristic and metaheuristic algorithms are often preferred to find sub-optimal solutions within an acceptable computation

time.

# Solving the CTSP via TSP methods

#### Transformation of the CTSP to the TSP 3.1

As the literature review shows, a number of dedicated solution approaches have been developed to solve the CTSP. However, one observes that these approaches have difficulty producing robustly and consistently high-quality solutions for large-scale CTSP instances with tens of thousands of vertices. Moreover, the best performing CTSP methods (e.g., VNRDGILS (Mestria, 2018), HHGILS (Mestria, 2016), and GPR1R2 (Mestria et al., 2013)) are computationally expensive (e.g., requiring 1080 seconds to find good solutions for instances with  $1173 \le n \le 2000$ ).

On the other hand, problem transformation has been highly successful in solving several difficult optimization problems such as the latin square completion problem via graph coloring (Jin and Hao, 2019) and the winner determination problem via weighted maximum cliques (Wu and Hao, 2015). It is known that the CTSP can be transformed to the conventional TSP (Chisman, 1975). Therefore, in principle, the CTSP can be solved by any TSP algorithm. However, to our knowledge, no computational study on using problem transformation to solve the CTSP has been presented in the literature. This work fills the gap by exploring the problem transformation approach of Chisman (1975) and testing three representative state-of-the-art TSP solvers including both exact and inexact solution approaches.

The basic idea of transforming the CTSP to the TSP is to add a large artificial cost M to all inter-cluster edges in order to force the salesman to visit all the cities within each cluster before leaving it.

Given a CTSP instance G = (V, E) with distance matrix C, we define a TSP instance G' = (V', E') with distance matrix C' as follow.

- Define V = V' and E = E'. Define the travel distance  $c'_{ij}$  in G' by

$$c'_{ij} = \begin{cases} c_{ij} + M & \text{if } i \text{ and } j \text{ belong to different clusters} \\ c_{ij} & \text{otherwise} \end{cases}$$

Obviously, if the value of M is sufficiently large, then the best Hamiltonian cycle in G' is a feasible CTSP solution in G, in which the vertices of each cluster are visited contiguously.

**Property.** An optimal solution to the TSP instance corresponds to an optimal solution to the original CTSP instance.

**Proof.** Let S' and S be the optimal solutions of the TSP instance G' and the original CTSP instance G, respectively. Let m be the number of clusters of G. To minimize the total travel cost, there are only m inter-cluster edges in S'. Therefore, S' is a feasible CTSP solution for G and satisfies the following relation:

$$f(S') = f(S) + m \times M$$

Obviously, S' corresponds to S by subtracting the constant  $m \times M$ .

#### 3.2 Solution methods for the TSP

There are numerous solution methods for the TSP. In this work, we adopt three very powerful TSP solvers whose codes are publicly available, including one exact solver (Concorde (Applegate et al., 2006a)) and two inexact (heuristic) solvers (LHK-2 (Helsgaun, 2009) and GA-EAX (Nagata and Kobayashi, 2013)).

Notice that the TSP instance converted from a CTSP instance has a particular feature that the vertices are grouped into clusters and the distance between each pair of vertices within a same cluster is in general small, while this distance is large for two vertices from different clusters. Along with the presentation of the TSP solvers, we discuss their suitability for solving such clustered instances each time this is appropriate.

#### 3.2.1 Exact Concorde solver

Concorde is an advanced exact TSP solver for the symmetric TSP based on Branch-and-Bound and problem specific cutting plane methods (Applegate et al., 2006a). It makes use of a specifically designed QSopt linear programming solver. According to Hoos and Stützle (2014), Concorde is the best performing exact algorithm for the TSP. As shown in Applegate et al. (2006b), Concorde can solve benchmark instances from TSPLIB with up to 1000 vertices to optimality within a reasonable computation time and it also solves large TSP instances at the cost of a long computation time.

The run time behavior of Concorde has been investigated essentially on random uniform instances. For instance, Applegate et al. (2006b) investigated the run time required by Concorde for solving random uniform instances and

indicated that the run time increases as an exponential function of instance size |V|. Hoos and Stützle (2014) further demonstrated that the median run time required by Concorde scales with instance size |V| of the form  $ab^{\sqrt{|V|}}$  ( $a\approx 0.21, b\approx 1.24$ ) on the widely studied class of uniform random TSP instances. To our knowledge, no study has been reported concerning the behavior of Concorde on sharply clustered instances. As a result, the current study will provide useful information on this issue.

#### 3.2.2 Lin-Kernighan based heuristic solver

According to the TSP literature, a majority of the best performing TSP heuristic algorithms is based on the Lin-Kernighan (LK) heuristic (Lin and Kernighan, 1973) and its extensions. The LK heuristic is a variable-depth k-opt local search procedure, where the k-opt neighborhood is partially searched with a smart pruning strategy. LK explores the most promising neighbors within the k-opt neighborhood, that is, the set of feasible tours obtained by removing k edges and adding other k edges such that the resulting tour is feasible. Several improved versions of the basic LK heuristic have been introduced within the iterated local search framework (e.g., Applegate et al. (2003); Helsgaun (2000, 2009); Martin et al. (1991)).

Among these iterated LK algorithms, Helsgaun's LKH (Helsgaun, 2000, 2009) is the uncontested state-of-the-art heuristic TSP solver. Helsgaun (2000) developed an iterated version of LK together with an efficient implementation of the LK algorithm, known as the Lin-Kernighan-Helsgaun (LKH-1) heuristic, where a 5-opt move is used as the basic move to broaden the search and an  $\alpha$ -measure method based on sensitivity analysis of minimum spanning trees is used to restrict the search to relative few of the  $\alpha$ -nearest neighbors of a vertex to speed up the search process. Later, Helsgaun (2009) further extended LKH-1 by developing a highly effective implementation of the k-opt procedure (called LKH-2), which eliminated many of the limitations and shortcomings of LKH-1. Furthermore, LKH-2 specially extended the data structures of LKH-1 to solve very large TSP instances. The main features of LKH-2 include (1) using sequential and non-sequential k-opt moves, (2) using several partitioning procedures to partition a large TSP instance into smaller subproblems, (3) using a tour merging procedure to generate a better solution from two or more local optimum solutions, and (4) applying a backbone-guided search to guide the local search to make biased local perturbations. LKH-2 is considered to be one of most effective heuristic methods for finding very high-quality solutions for various large TSP instances (Dubois-Lacoste et al., 2015).

However, the LK algorithm and any LK-based algorithms require much longer running times on clustered instances of the TSP than on uniformly distributed instances (Neto, 1999). The main reason why the LK heuristic stumbles on

clustered instances is that relatively large inter-cluster edges serve as bait edges. During the LK search, when removing such a bait edge, the LK heuristic is tricked into long and often fruitless searches. More precisely, each time an edge bridging two clusters is removed, the cumulative gain rises enormously, and the procedure is encouraged to perform very deep searches. To alleviate the problem, a cluster compensation technique was proposed in Neto (1999) for the Lin-Kernighan heuristic to limit its performance degradation. Helsgaun (2009) showed that the LKH-2 algorithm performs significantly worse on sharply clustered instances than on uniform random instances. To remedy this difficulty, Helsgaun (2014) considered the unusual structure of clustered instances, and adjusted the parameter settings of LKH-2 to better solve the clustered instances. The resulting solver is named CLKH, which is used in this study.

# 3.2.3 Edge assembly crossover based genetic algorithm

Population-based evolutionary algorithms are another well-known approach for the TSP. A popular example is the powerful genetic algorithm introduced by Nagata and Kobayashi (2013). This algorithm (called GA-EAX, see Algorithm 1) is characterized by its powerful edge assembly crossover (EAX) operator introduced in Nagata and Kobayashi (1997); Nagata and Soler (2012) with an efficient implementation and a cost-effective selection strategy for maintaining population diversity.

# **Algorithm 1** GA-EAX for the CTSP

**Require:** TSP instance G, population size p; number of offspring solutions r generated from each parent pair

```
Ensure: best solution S^*
 1: POP = \{P_1, P_2, ..., P_p\} \leftarrow \text{Initial\_Population}(G)
 2: while stopping condition is not met do
        Randomly shuffle the solutions in POP
 3:
        for i = 1, 2, ..., p do
 4:
           S_1 \leftarrow P_i, S_2 \leftarrow P_{i+1} / * \text{Note: } P_{p+1} = P_1 * /
 5:
           (o_1,...,o_r) \leftarrow \text{EAX}(S_1,S_2)
 6:
 7:
           P_i \leftarrow \text{Select\_Best}(o_1, ..., o_r, S_1)
 8:
        end for
 9: end while
10: S^* \leftarrow \text{Best}(POP)
11: Return S^*
```

The key EAX operator generates, from two high-quality tours (parents), one offspring tour by first inheriting the edges from the parents to construct disjoint subtours and then connecting the subtours with new edges in a greedy fashion (similar to building a minimal spanning tree). Let  $S_A$  and  $S_B$  be the parents, EAX operates as follows (see Fig. 2 for an example):

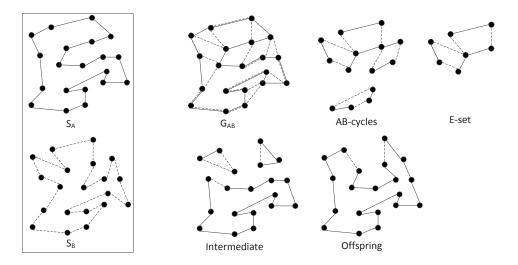


Fig. 2. Illustrative example of the EAX crossover operator

- (1) Generate an undirected multigraph defined as  $G_{AB} = (V, E_A \cup E_B)$ , where  $E_A$  and  $E_B$  are the sets of edges of parents  $S_A$  and  $S_B$ , respectively.
- (2) Extract all AB-cycles from  $G_{AB}$ . An AB-cycle is defined as a cycle in  $G_{AB}$ , such that edges of  $E_A$  and edges of  $E_B$  are alternately linked.
- (3) Construct an E-set by selecting AB-cycles according to a given selection strategy (e.g., single, k-multiple, block and block2 (Nagata and Kobayashi, 2013)), where an E-set is a set of AB-cycles.
- (4) Copy parent  $S_A$  to an intermediate solution o. Then, remove the edges of  $E_A$  in the E-set from o and add those of  $E_B$  in the E-set to o. This leads to an intermediate solution o with one or more subtours.
- (5) Connect all the subtours in o with new short edges to generate a complete tour (a feasible offspring solution) by using a greedy heuristic.

Note that different versions of EAX can be developed by using different selection strategies of AB-cycles for constructing E-sets. The GA-EAX algorithm employs the single and block2 strategies to generates offspring solutions from parent solutions. To maintain a healthy population diversity, GA-EAX also uses an edge entropy measure to select the solution to be used to replace a parent in the population.

Other studies (e.g., Hains et al. (2012)) also indicated the usefulness of edge-assembly-like crossovers for solving clustered instances of the TSP. As shown in the next section, the EAX-based genetic algorithm performs remarkably well on all the clustered instances transformed from the CTSP.

# 4 Computational experiments

In this section, we evaluate the capacity of the TSP solvers presented in Section 3.2 to solve the CTSP via its transformation to the TSP. For this purpose, we examine their qualitative performances and run time efficiencies on various benchmark instances and make comparisons with the best dedicated CTSP algorithms in the literature.

#### 4.1 Benchmark instances

Our computational assessments are based on three sets of 73 benchmark instances with 101 to 24,978 vertices. Sets 1 and 2 include 20 medium instances ( $101 \le |V| \le 1000$ ) and 15 large instances ( $1173 \le |V| \le 2000$ ), which are classical and widely used in the CTSP literature (e.g., Mestria et al. (2013); Mestria (2016, 2018)). Set 3 includes 38 large GTSP instances ( $1000 \le |V| \le 24,978$ ) from Helsgaun (2014).

Sets 1 and 2 (35 instances): These instances belong to the following six types: (1) instances taken from the TSPLIB (Reinelt, 1991) where the clusters are generated by using a k-means clustering algorithm; (2) instances created from a selection of classic TSP instances (Johnson and McGeoch, 2007), where the clusters are created by grouping the vertices in geometric centers; (3) instances generated by using the Concorde interface (Applegate et al., 2006a); (4) instances generated using the layout proposed in Laporte and Palekar (2002); (5) instances similar to type 2, but generated with different parameters; (6) instances adapted from the TSPLIB (Reinelt, 1991), where the rectangular floor plan is divided into several quadrilaterals and each quadrilateral corresponds to a cluster. These instances are available at http://www2.ic.uff.br/~labic/conteudo/instance/.

Set 3 (38 instances): These large instances have 1000 to 24,978 vertices and come from GTSPLIB for the generalized traveling salesman problem (GTSP). They were generated from TSP instances by using Fischetti et al.'s clustering algorithm (Fischetti et al., 1997) and tested in Helsgaun (2014) by considering them as CTSP instances. These instances are available at http://www.ruc.dk/~keld/research/CLKH. In Helsgaun (2014), six very large instances with 31,623 to 85,900 vertices were also tested. We ignore these instances, because they are too large for the exact Concorde solver and the GA-EAX solver stops abnormally when solving these instances.

# 4.2 TSP solvers and experimental protocol

For our study, we employed three representative TSP solvers presented in Section 3.2, which are among the most powerful methods for the TSP in the literature.

- Exact Concorde TSP solver <sup>1</sup>: We used version Concorde-03.12.19 and ran the solver with its default parameter setting with a cutoff time of 24 CPU hours per instance.
- Inexact CLKH solver  $^2$ : We used the version CLKH-1.0 which is based on the latest version  $2.0.9^3$  of LKH-2. The default parameter setting given in Helsgaun (2014) was adopted to run CLKH. Notice that to reduce its run time, the maximum number of trials (iterations) is set to 1000 in CLKH, while this number is set to n (instance size) by default in LKH-2.
- Inexact GA-EAX TSP solver <sup>4</sup>: We used GA-EAX with its default parameter setting given in Nagata and Kobayashi (2013): p = 300, r = 30 and GA-EAX terminates if the difference between the average tour length and the shortest tour length in the population is less than 0.001. Following Kerschke et al. (2018); Kotthoff et al. (2015), we reset the random seed for GA-EAX for each run (which was set to a fixed value in the official implementation).

The experiments were carried out on a computer running Linux operating system with an Intel E5-2670 processor (2.8 GHz and 4G RAM). Given the stochastic nature of CLKH and GA-EAX, we ran each algorithm 10 times for each instances while the deterministic Concorde TSP solver was run one time to solve each instance.

# 4.3 Computational results and comparison of popular TSP solvers

Our computational studies aim to answer the following questions: How do state-of-the-art *exact* TSP solvers perform on clustered instances converted from the CTSP? How do state-of-the-art *inexact* (heuristic) TSP solvers perform on clustered instances converted from the CTSP?

The results of the three TSP solvers (Concorde, CLKH, GA-EAX) on the 20 medium and 15 large CTSP benchmark instances are summarized in Table 1 (Set 1) and Table 2 (Set 2). Columns 1 to 3 show the basic information of each

http://www.math.uwaterloo.ca/tsp/concorde/index.html

http://www.ruc.dk/~keld/research/CLKH

http://akira.ruc.dk/~keld/research/LKH/

<sup>4</sup> https://github.com/sugia/GA-for-TSP

instance: the instance name (Instance), the number of vertices (|V|) and the number of clusters (m). Column 4 gives the optimal objective value reported by the exact Concorde TSP solver, followed by the required run time in seconds. For both the CLKH and GA-EAX solvers, we show the best  $(Gap_{best})$  and average  $(Gap_{avg})$  results over 10 independent runs in the form of the percentage gap to the optimal solution, as well as the average run time in seconds. If the best solution over 10 independent runs equals the optimal solution obtained with the exact Concorde TSP solver, the corresponding cell in column  $Gap_{best}$  shows '=' along with the number of runs that succeeded in finding the optimal solution. Finally, row 'Avg.' provides the average run time in seconds for each approach, and the average gap between the average objective values obtained with CLKH/GA-EAX and the optimal values obtained with the Concorde TSP solver.

Table 1 Computational results of the TSP solvers Concorde, CLKH and GA-EAX on medium CTSP instances (Set 1).

			Concor	de		CLKH		(	GA-EAX	
Instance	V	m	Opt.	t(s)	$Gap_{best}$	$Gap_{avg}$	t(s)	$Gap_{best}$	$Gap_{avg}$	t(s)
i-50-gil262	262	50	135431	1.9	=(10)	0.0000	1.3	=(10)	0.0000	1.7
10-lin318	318	10	529584	2.2	=(10)	0.0000	19.5	=(10)	0.0000	1.8
10-pcb $442$	442	10	537419	20.7	=(10)	0.0000	46.9	=(10)	0.0000	6.3
C1k.0	1000	10	132521027	21.9	=(9)	0.0001	128.6	=(10)	0.0000	16.3
C1k.1	1000	10	129128125	22.3	=(10)	0.0000	70.6	=(10)	0.0000	14.3
C1k.2	1000	10	142784000	69.9	0.0009	0.0009	244.6	=(9)	0.0001	17.2
300-6	300	6	8934	4.4	=(10)	0.0000	30.2	=(10)	0.0000	3.5
400-6	400	6	9045	6.7	=(10)	0.0000	26.7	=(10)	0.0000	4.4
700-20	700	20	41425	29.9	=(10)	0.0000	200.0	=(10)	0.0000	10.2
200-4-h	200	4	62777	0.6	=(10)	0.0000	5.4	=(10)	0.0000	0.9
200-4-x1	200	4	60574	1.1	=(10)	0.0000	6.5	=(10)	0.0000	0.9
600-8-z	600	8	128891	9.9	=(10)	0.0000	48.2	=(10)	0.0000	5.3
600-8-x2	600	8	128891	4.8	=(10)	0.0000	48.2	=(10)	0.0000	5.3
300-5-108	300	5	67760	1.2	=(10)	0.0000	8.5	=(10)	0.0000	2.0
300-20-111	300	20	309739	1.8	=(10)	0.0000	6.0	=(10)	0.0000	2.0
500-15-306	500	15	194818	2.6	=(10)	0.0000	37.1	=(10)	0.0000	5.2
500-25-308	500	25	365447	4.4	=(10)	0.0000	10.1	=(10)	0.0000	5.4
25-eil $101$	101	25	23671	0.5	=(10)	0.0000	0.4	=(10)	0.0000	0.8
42-a280	280	42	129645	2.3	=(10)	0.0000	2.4	=(10)	0.0000	1.7
144-rat783	783	144	914228	70.2	=(10)	0.0000	14.6	=(10)	0.0000	9.4
Avg.		·		14.0		0.0001	47.8		0.0000	5.7

From Tables 1-2, we can make the following observations:

First, the exact Concorde TSP solver performs very well on these 35 instances and is able to solve all of them exactly. Specifically, the 20 medium instances can be solved easily in a short run time (an average of about 14 seconds). The 15 large instances are more difficult and the run time needed to solve these instances increases considerably (an average of 1133.8 seconds, reaching 7214.3 seconds for the most difficult instance).

Second, the CLKH solver performs globally very well on these 35 instances. For the 20 medium instances, CLKH attains all the optimal solutions but one with an average run time of 47.8 seconds. For the 15 large instances, CLKH

Table 2 Computational results of the TSP solvers Concorde, CLKH and GA-EAX on large CTSP instances (Set 2).

			Conco	rde		CLKH		(	GA-EAX	
Instance	V	m	Opt.	t(s)	$Gap_{best}$	$Gap_{avg}$	t(s)	$Gap_{best}$	$Gap_{avg}$	t(s)
49-pcb1173	1173	49	61600	5638.3	0.6250	1.0519	1065.8	=(4)	0.0326	35.0
100-pcb1173	1173	100	63382	588.3	=(7)	0.0066	63.2	=(8)	0.0013	32.5
144-pcb1173	1173	144	62142	38.4	=(10)	0.0000	25.8	=(10)	0.0000	18.6
10-nrw1379	1379	10	58783	562.9	=(10)	0.0000	174.9	=(6)	0.0070	26.8
$12\text{-}\mathrm{nrw}1379$	1379	12	59129	58.5	=(10)	0.0000	39.7	=(9)	0.0007	27.6
1500-10-503	1500	10	11116	65.5	=(5)	0.0225	603.6	=(10)	0.0000	28.4
1500-20-504	1500	20	15698	40.7	=(10)	0.0000	167.9	=(5)	0.0172	34.5
1500-50-505	1500	50	22900	67.0	=(7)	0.0476	178.8	=(5)	0.0044	35.1
1500-100-506	1500	100	29799	108.7	=(6)	0.0228	58.3	=(8)	0.0020	39.5
1500-150-507	1500	150	34068	114.7	=(10)	0.0000	44.4	=(10)	0.0000	32.3
2000-10-a	2000	10	105360	7214.3	0.0038	0.0155	401.9	0.0826	0.1167	45.3
2000-10-h	2000	10	33708	812.7	=(9)	0.0006	229.9	=(10)	0.0000	35.6
2000-10-z	2000	10	33509	200.9	=(10)	0.0000	160.1	=(9)	0.0003	37.3
2000-10-x1	2000	10	33792	1325.4	=(4)	0.0213	485.3	=(6)	0.0136	35.6
2000-10-x2	2000	10	33509	170.9	=(10)	0.0000	160.1	=(10)	0.0000	39.6
Avg.				1133.8		0.0793	257.3		0.0131	33.6

reaches the optimal solutions for 13 instances with an average run time of 257.3 seconds.

Third, the GA-EAX solver performs remarkably well by attaining the optimal values for all 35 instances but one. For the 20 medium instances, GA-EAX consistently hits the optimal solutions for each of its 10 run (except for one instance for which it has a hit of 9 out of 10). The average run time is only 5.7 seconds for the medium instances and 33.6 seconds for the large instances. Compared to Concorde and CLKH, GA-EAX is thus extremely time efficient. Moreover, contrary to the Concorde and CLKH solvers, the computation time required by GA-EAX remains very stable across the instances of the same set, indicating a high robustness and scalability of this solver.

Table 3 presents the results of the three TSP solvers on the 38 large GTSP instances of Set 3. Notice that the Concorde solver failed to exactly solve 17 instances in 24 hours, the corresponding cell (in parentheses) in column 'Optimum' indicates the best tour length (best upper bound) found by CLKH and GA-EAX. In this case, the percentage gaps  $(Gap_{best}$  and  $Gap_{avg})$  are calculated by using the best bound, and column  $Gap_{best}$  shows '=' the number of runs for an algorithm to find the best bound.

From Table 3, we can make the following observations. First, Concorde manages to optimally solve 21 large GTSP instances with up to 3162 vertices with a run time ranging from 17.4 seconds to 45008.4 seconds while its solution time is not completely consistent with the size of the problem instances. For the 21 instances that can be solved exactly by Concorde, CLKH attains 15 best upper bounds, while GA-EAX reaches all best upper bounds in less computing time. Second, for most of the instances with |V| < 10,000, compared with CLKH, GA-EAX has a better performance both in terms of solution

Table 3 Computational results of the TSP solvers Concorde, CLKH and GA-EAX on large GTSP instances (Set 3).

						CLKH			GA-EAX	
Instance	V	m	Optimum	Concorde's run-time	$Gap_{best}$	$Gap_{avg}$	t(s)	$Gap_{best}$	$Gap_{avg}$	t(s)
10C1k.0	1000	10	12139627	23.5	=(9)	0.0016	194.5	=(10)	0.0000	16.1
$200\mathrm{C1k.0}$	1000	200	11929315	17.4	=(10)	0.0000	64.7	=(10)	0.0000	15.6
$200\mathrm{E}1\mathrm{k}.0$	1000	200	24468822	66.2	=(8)	0.0008	27.7	=(10)	0.0000	15.1
49usa $1097$	1097	49	77583052	51.1	=(7)	0.0069	128.6	=(10)	0.0000	23.7
235pcb1173	1173	235	59796	65.5	=(9)	0.0151	36.4	=(10)	0.0000	16.4
259d1291	1291	259	55962	8402.5	0.0286	0.0484	51.7	=(7)	0.0064	17.3
261 rl1 304	1304	261	261132	19.2	=(10)	0.0000	18.7	=(10)	0.0000	7.5
265 rl1323	1323	265	280004	3361.3	0.0114	0.0381	18.9	=(8)	0.0019	10.2
276nrw1379	1379	276	60473	234.4	=(3)	0.0223	30.8	=(10)	0.0000	30.7
280fl1400	1400	280	20229	6108.5	=(3)	0.0900	504.7	=(8)	0.0178	21.5
287u1432	1432	287	162151	23029.9	=(8)	0.0136	111.6	=(10)	0.0000	26.8
316fl1577	1577	316	23023	1179.6	=(10)	0.0000	183.0	=(2)	0.2332	17.2
331d1655	1655	331	65871	142.9	=(3)	0.0797	51.8	=(7)	0.0029	24.6
350 vm 1748	1748	350	348244	230.9	=(2)	0.0371	88.2	=(10)	0.0000	25.7
364 u 1817	1817	364	61879	5675.7	=(1)	0.0739	77.7	=(6)	0.0050	31.8
378rl1889	1889	378	323040	461.5	=(1)	0.1197	29.0	=(10)	0.0000	18.1
421d2103	2103	421	(91637)	-	=(2)	0.0598	112.7	=(10)	0.0000	32.8
431u2152	2152	431	(69876)	-	=(2)	0.0215	98.5	=(10)	0.0000	37.0
464u2319	2319	464	(246707)	-	=(10)	0.0000	703.2	=(3)	0.0167	84.9
479 pr 2392	2392	479	397707	1267.5	=(4)	0.0223	102.1	=(10)	0.0000	38.0
608pcb3038	3038	608	146351	45008.4	0.0014	0.0256	115.5	=(4)	0.0018	83.2
31C3k.0	3162	31	20058457	912.6	0.0144	0.0637	249.2	=(5)	0.0211	111.6
633C3k.0	3162	633	20158425	1650.4	0.0207	0.0869	163.5	=(8)	0.0011	98.0
633E3k.0	3162	633	42697510	5239.0	0.0036	0.0226	105.7	=(3)	0.0052	115.0
759fl3795	3795	759	(29582)	-	=(9)	0.0068	464.0	0.2637	0.3729	53.9
893fnl4461	4461	893	(193834)	-	=(2)	0.0163	139.0	=(8)	0.0004	236.6
1183rl5915	5915	1183	(599096)	-	0.0212	0.1666	204.3	=(9)	0.0006	146.6
1187rl5934	5934	1187	(588074)	-	0.0126	0.1256	251.6	=(5)	0.0033	156.1
1480pla7397	7397	1480	(23926551)	-	0.0035	0.0213	1104.7	=(2)	0.0078	388.2
100C10k.0	10000	100	(36352580)	-	=(1)	0.6815	1877.4	0.0525	0.4872	2318.7
2000C10k.0	10000	2000	(34574383)	-	0.0369	0.2590	730.6	=(1)	0.0139	992.9
2000E10k.0	10000	2000	(75506665)	=	0.0112	0.0281	635.8	=(1)	0.0013	1320.0
2370rl11849	11849	2370	(977472)	-	0.0081	0.0477	757.1	=(1)	0.0028	1051.9
702usa13509	13509	2702	(20836160)	-	0.0118	0.0185	1028.6	=(1)	0.0012	2154.0
811brd14051	14051	2811	(496827)	-	0.0125	0.0213	944.7	=(1)	0.0024	2454.9
3023d15112	15112	3023	(1658091)	-	0.0220	0.0296	1193.3	=(1)	0.0019	3864.0
3703d18512	18512	3703	(683839)	=	0.0209	0.0328	1561.9	=(1)	0.0019	4306.8
.996sw24978	24978	4996	(893042)	=	0.0237	0.0369	2076.3	=(1)	0.0008	5706.2
Avg.			. ,			0.0616	427.3		0.0319	686.0

quality and computation time. For the instances with  $10,000 \le |V| \le 24,978$ , the solution quality of GA-EAX is better than that of CLKH in most cases, while requiring more computation time.

To sum up, the exact Concorde solver is very efficient for the instances with up to 1000 vertices (order of seconds) and can even find optimal solutions for instances with up to some 3000 vertices at a price of more run time (order of minutes to hours). For larger instances, both inexact solvers (CLKH and GA-EAX) are reliable alternatives to find optimal or sub-optimal solutions with some advantages for GA-EAX. These heuristic solvers also perform very well on smaller instances.

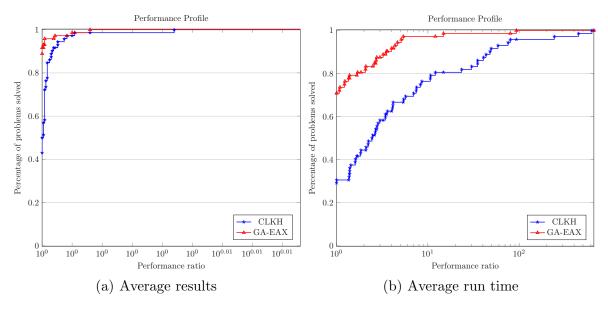


Fig. 3. Performance profiles comparing solution quality and computing time.

To deepen our computational study, we call upon to the performance profile, an analytic tool for evaluating the performances of multiple compared optimization algorithms (Dolan and Moré, 2002). The performance profile uses a cumulative distribution function for a performance metric, such as run time, objective function values, number of iterations, and so on. Precisely, let S be a set of algorithms and P be a set of problem instances. For a given performance metric  $f_{s,p}$  (that is the performance of algorithm  $s \in S$  solving instance  $p \in P$ ), the performance ratio is defined by  $r_{s,p} = \frac{f_{s,p}}{\min\{f_{a,p}:a\in S\}}$ . Then, for each algorithm  $s \in S$ , the performance function is given by  $\rho_s(\tau) = \frac{|\{p \in P: r_{s,p} \leq \tau\}|}{|P|}$ . Thus, the value of  $\rho_s(1)$  corresponds to the fraction of problem instances that algorithm s can achieve many times the performance of the best algorithm (meaning the probability that the algorithm s will win over the rest of the compared algorithms). For a large value  $\tau$ , the value of  $\rho_s(\tau)$  indicates a high robustness of algorithm s.

To make a fair and meaningful comparison with this tool, we focus on the two inexact solvers CLKH and GA-EAX and run each solver 10 times on each of the 73 instances. We use the software 'perprof-py' (Siqueira et al., 2016) to draw the performance profiles (see Figure 3) where the quality of the solution is measured by the average objective value and average run time. These performance profiles tend to show an advantage of GA-EAX over CLKH for solving these clustered instances with up to 24,978 vertices.

# 4.4 TSP solvers v.s. state-of-the-art CTSP heuristics

In Section 4.3, we observed that the exact Concord TSP solver and the inexact CLKH and GA-EAX TSP solvers are powerful tools for solving clustered TSP instances converted from the CTSP. We now answer the following question: Do these general TSP solvers compete well with state-of-the-art CTSP heuristics specially designed for the problem?

Table 4 List of the reference algorithms for the CTSP

Algorithm name	Reference	Search strategy
VNRDGILS	Mestria (2018)	A hybrid heuristic based on GRASP, ILS and VNRD
HHGILS	Mestria (2016)	A hybrid heuristic based on GRASP, ILS and VND
GPR1R2	Mestria et al. (2013)	A GRASP with Path Relinking PR1 and PR2
GPR1	Mestria et al. (2013)	A GRASP with Path Relinking PR1
GPR2	Mestria et al. (2013)	A GRASP with Path Relinking PR2
GPR3	Mestria et al. (2013)	A GRASP with Path Relinking PR3
GPR4	Mestria et al. (2013)	A GRASP with Path Relinking PR4
GRASP	Mestria et al. (2013)	A traditional GRASP heuristic
TLGA	Ding et al. (2007)	A two-level genetic algorithm

For this purpose, we adopt GA-EAX as our representative TSP solver and compare it with three best performing CTSP heuristics in the literature: VN-RDGILS (Mestria, 2018), HHGILS (Mestria, 2016), and GPR1R2 (Mestria et al., 2013). Indeed, according to the experimental studies reported in Mestria et al. (2013); Mestria (2016, 2018), these three heuristics perform the best among the recent CTSP heuristics available in the literature (see Table 4). This study is based on the 35 medium and large instances of Sets 1 and 2 (no results for the three CTSP heuristics are available on the large GTSP instances of Set 3).

Table 5 provides the comparative results of the GA-EAX TSP solver along with the results reported by the three CTSP algorithms on the medium and large instances. For each instance and algorithm, columns ' $f_{best}$ ', ' $f_{avg}$ ' and t(s) show respectively the best objective value over 10 independent runs, the average objective value and the average run time in seconds. Furthermore, the row 'Avg.' shows the average performances for each compared algorithm, including the average percentage gap of the best/average result to the optimal result obtained with the Concorde TSP solver and the average run time in seconds. To determine whether there exists a statistically significant difference in performance between the GA-EAX TSP solver and each CTSP algorithm in terms of best and average results, the p-values from the Wilcoxon signed-rank tests are given in the last row of Table 5. Entries with "-" mean that the corresponding results are not available in the literature. The best objective values obtained by the compared algorithms are indicated in bold if they attain the optimal solution. Notice that the results of the CTSP algorithms (VNRDG-ILS, HHGILS and GPR1R2) correspond to 10 executions per instance on a computer with 2.83 GHz Intel Core 2 CPU and 8 GB RAM and the time limit

Table 5: Comparative results between the GA-EAX TSP solver and three CTSP algorithms on medium and large CTSP instances.

				GA-EAX		Λ	VNRDGILS			HHGILS			GPR1R2	
Instance	<u> </u>	u u	$f_{best}$	favg	t(s)	$f_{best}$	favg	t(s)	$f_{best}$	favg	t(s)	fbest	favg	t(s)
i-50-gil262	262	20	135431	135431.0	1.7	135483	135510.2	720.0	135510	135578	720.0	-	-	-
10-lin318	318	10	529584	529584.0	1.8	530604	530871.4	720.0	530283	530817.9	720.0	530443	532697.9	720.0
10-pcb442	442	10	537419	537419.0	6.3	538309	538903.4	720.0	538958	539988.3	720.0	540043	543104.2	720.0
C1k.0	1000	10	132521027	132521027.0	16.3	133260549	133490775.9	720.0	133287594	133776274.1	720.0	133490776	133708187.6	720.0
C1k.1	1000	10	129128125	129128125.0	14.3	129877874	130035540.2	720.0	129825403	130206778.3	720.0	130193590	130391693.5	720.0
C1k.2	1000	10	142784000	142784188.4	17.2	143321630	143481489.6	720.0	143278093	143525149.6	720.0	,	,	,
300-6	300	9	8934	8934.0	3.5	8935	8941.1	720.0	8934	8942.9	720.0	8959	8985.3	720.0
400-6	400	9	9045	9045.0	4.4	9053	9062.3	720.0	9051	9063.2	720.0	,	,	,
700-20	200	20	41425	41425.0	10.2	41456	41489.7	720.0	41452	41485.6	720.0	41540	41573.3	720.0
200-4-h	200	4	62777	62777.0	6.0	62867	63058.3	720.0	62804	63058.3	720.0	62994	63710.2	720.0
200-4-x1	200	4	60574	60574.0	6.0	60637	60796.2	720.0	60931	61378.5	720.0	,	•	
z-8-009	009	œ	128891	128891.0	5.3	129468	129862.7	720.0	129416	129928.6	720.0	130459	131235.1	720.0
600-8-x2	009	œ	128891	128891.0	5.3	129246	129533.9	720.0	129246	129691.5	720.0	,	,	,
300-5-108	300	ъ	67760	67760.0	2.0	99449	67868.7	720.0	67814	67930.5	720.0	,	•	
300-20-111	300	20	309739	309739.0	2.0	310146	310270.9	720.0	310209	310427	720.0	309928	310551.9	720.0
500-15-306	200	15	194818	194818.0	5.2	194946	195201.5	720.0	195202	195438.1	720.0	,		,
500-25-308	200	25	365447	365447.0	5.4	365717	365937.8	720.0	365828	366085	720.0	366232	366785.7	720.0
25-eil101	101	25	23671	23671.0	8.0	23673	23685.2	720.0	23678	23690	720.0	23676	23711.3	720.0
42-a280	280	42	129645	129645.0	1.7	129729	129755.2	720.0	129716	129833.2	720.0	,		,
144-rat783	783	144	914228	914228.0	9.4	915088	915179.8	720.0	915180	915363.2	720.0	915547	915913.7	720.0
49-pcb1173	1173	49	61600	61620.1	35.0	65750	66487.7	1080.0	67043	68260.7	1080.0	70651	73311.9	1080.0
100-pcb1173	1173	100	63382	63382.8	32.5	88208	69383.2	1080.0	68786	70640.8	1080.0	72512	74871.7	1080.0
144-pcb1173	1173	144	62142	62142.0	18.6	68414	68941.4	1080.0	66830	69084.3	1080.0	72889	74621.6	1080.0
10 - nrw 1379	1379	10	58783	58787.1	26.8	63951	64895.9	1080.0	63620	64643.9	1080.0	66747	68955.8	1080.0
12 - nrw1379	1379	12	59129	59129.4	27.6	62893	63532.3	1080.0	63558	64741.6	1080.0	66444	69141.2	1080.0
1500-10-503	1500	10	11116	11116.0	28.4	11969	12103.0	1080.0	11986	12109.5	1080.0	12278	12531.4	1080.0
1500-20-504	1500	20	15698	15700.7	34.5	16678	16867.4	1080.0	17107	17315.7	1080.0	17252	17589.1	1080.0
1500-50-505	1500	20	22900	22901.0	35.1	24631	24803.6	1080.0	25264	25558.9	1080.0	25124	25761.5	1080.0
1500-100-506	1500	100	29799	29799.6	39.5	32474	32616.8	1080.0	32260	33760.6	1080.0	33110	33692.7	1080.0
1500-150-507	1500	150	34068	34068.0	32.3	37357	38251.1	1080.0	37658	38433.1	1080.0	38767	39478.0	1080.0
2000-10-a	2000	10	105447	105483.0	45.3	115779	116897.3	1080.0	116254	116881.4	1080.0	116473	118297.5	1080.0
2000-10-h	2000	10	33708	33708.0	35.6	36806	38351.8	1080.0	36447	37305.1	1080.0	37529	38861.8	1080.0
2000-10-z	2000	10	33509	33509.1	37.3	36815	38035.7	1080.0	37059	37443.7	1080.0	37440	38765.9	1080.0
2000-10-x1	2000	10	33792	33796.6	35.6	36783	37488.6	1080.0	36752	37704.0	1080.0	37262	39253.1	1080.0
2000-10-x2	2000	10	33509	33509.0	39.6	37132	38240.6	1080.0	36660	37117.1	1080.0	37704	38699.5	1080.0
Avg.			0.00	0.01	17.7	3.79	4.62	874.3	3.94	4.96	874.3	86.9	8.94	920.0
p-value						2.477e-7	2.477e-7		3.651e-7	2.477e-7				

per run was set to 720 seconds for medium instances and 1080 seconds for large instances.

Table 6 Statistical results for the GA-EAX TSP solver and three state-of-the-art CTSP algorithms on Set 1 (medium instances) and Set 2 (large instances). Dominating values are indicated in bold.

		GA-EAX	VNRDGILS	HHGILS	GPR1R2
Set 1	Optimal solutions	20/20	0/20	1/20	0/20
	Average $Gap_{best}/Gap_{avg}(\%)$	0.00/0.00	0.18/0.30	0.21/0.40	0.39/0.73
	Average time (s)	5.7	720.0	720.0	720.0
Set 2	Optimal solutions	14/15	0/15	0/15	0/15
	Average $Gap_{best}/Gap_{avg}(\%)$	0.00/0.01	8.61/10.39	8.92/11.04	12.25/15.51
	Average time (s)	33.6	1080.0	1080.0	1080.0

Table 6 summarizes the statistical results for each compared algorithm on the two sets of medium and large instances. The first row indicates the number of optimal solutions found by each approach. The average percentage gap of the best/average result from the optimal result is provided in row 'Average  $Gap_{best}/Gap_{avg}$ '. Finally, row 'Average time (s)' provides the average run time in seconds for each algorithm.

From Tables 5 and 6, we observe that the GA-EAX solver significantly outperforms the three CTSP algorithms on the medium and large instances in terms of both the best and the average results. For the large instance set, the improvement gaps between the results of GA-EAX and those of the CTSP methods are very high, ranging from 10.39% to 15.49%. Furthermore, in terms of the average run time, GA-EAX is about 30 to 130 times faster than the CTSP algorithms. The above results thus indicate that the GA-EAX TSP solver has a strong dominance over current best performing CTSP approaches in the literature. In addition, the small p-values (<0.05) from the Wilcoxon signed-rank tests further confirm the statistically significant difference of the compared results.

To have a finer analysis of the compared algorithms, Figure 4 provides boxplot graphs to compare the distribution and range of the average results for each compared algorithm, except GPR1R2 for the medium instances since its results on several medium instances are not available. In this figure, the average objective value  $f_{avg}$  of a given algorithm is normalized according to the relation  $y = 100*(f_{avg} - f_{opt})/f_{opt}$ , where  $f_{opt}$  is the optimal value. The plots in Figure 4 show clear differences in the distributions of the average results between GA-EAX and each compared CTSP heuristic, which further confirms the efficiency of the GA-EAX TSP solver with respect to these dedicated CTSP heuristics.

Finally, considering the results of the Concorde solver and the CLKH solver reported in Section 4.3, we conclude that these TSP solvers also dominate the

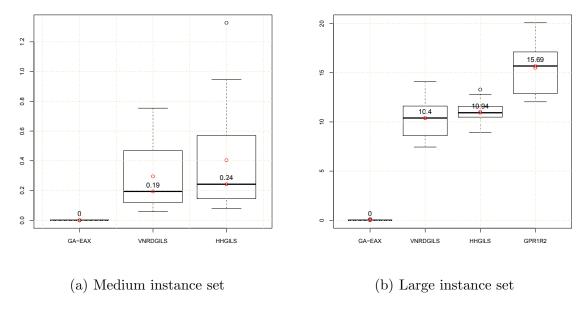


Fig. 4. Boxplots of the normalized average objective values for the medium instance set and large instance set.

current best CTSP algorithms in the literature.

#### 5 Discussion

We now provide additional explanations regarding the behaviors of the three TSP solvers. First, given the NP-hard nature of the CTSP and the exponential time complexity of the exact Concorde solver, it is expected that the exact Concorde solver reaches its limit when the instance to be solved reaches some size (about 3000 vertices for the studies instances). Indeed, when the search space becomes extremely large, the exact Branch-and-Bound search even equipped with the best problem specific cutting plane methods cannot effectively enumerate all candidate solutions. In fact, such a behavior has already been observed in previous studies on Concorde applied to classical TSP instances (Applegate et al., 2006b; Hoos and Stützle, 2014). Second, regarding the two heuristic solvers CLKH and GA-EAX, the CLKH solver exhibits a worse performance compared to GA-EAX. As discussed in Section 3.2.2, the underlying LK heuristic stumbles on clustered instances because relatively large intercluster edges serve as bait edges. With the presence of these bait edges, the LK heuristic may be tricked into long and often fruitless search trajectories. Third, the GA-EAX solver performs its search mainly with its edge assembly crossover, which inherits the edges of the parents to construct disjoint subtours and then connect the subtours. This crossover proves to be meaningful and helps the algorithm avoid local optimal traps. Once

again, the excellent behavior of GA-EAX on the CTSP instances is consistent with its performance on conventional TSP instances as shown in Nagata and Kobayashi (2013).

#### 6 Conclusion

This work presents the first extensive computational study on the transformation approach of solving the Clustered Traveling Salesman Problem with general TSP solvers. Based on the results from the exact Concorde solver and the heuristic CLKH and GA-EAX solvers on 20 medium ( $101 \le |V| \le 1000$ ) and 15 large ( $1173 \le |V| \le 2000$ ) CTSP benchmark instances and 38 large GTSP benchmark instances (with up to 24,978 vertices) available in the literature, we can draw the following conclusions.

- The exact Concorde solver can optimally solve all medium and large CTSP instances. It also solves exactly large GTSP instances with up to 3162 vertices in a reasonable time, but fails to solve larger GTSP instances in 24 hours. Its solution time is not completely consistent with the size of the problem instances.
- The heuristic CLKH and GA-EAX solvers perform very well both in terms of solution quality and computational efficiency. Both solvers have a good scalability, making them particularly suitable for solving very large instances with at least several thousands of vertices. For the tested instances with up to some 24,978 vertices, GA-EAX exhibits a better performance than CLKH.
- The general TSP solvers significantly dominate, both in terms of solution quality and computational efficiency, the current best performing CTSP heuristics specially designed for the problem. In particular, the TSP heuristics are several orders of faster than the state-of-the-art CTSP heuristics to find much better results.

This study indicates that the existing CTSP benchmark instances in the literature are not challenging for modern TSP solvers even if they remain difficult for the existing CTSP algorithms.

Finally, given the findings of this study, it would be interesting to investigate the problem transformation approach for solving other TSP variants that can be converted to the TSP or to a TSP variant for which effective algorithms are available.

# Acknowledgments

This work is partially supported by the National Natural Science Foundation Program of China [Grant No. 72122006].

#### References

- Anily, S., Bramel, J., Hertz, A., 1999. A 53-approximation algorithm for the clustered traveling salesman tour and path problems. Operations Research Letters 24, 29–35.
- Applegate, D., Bixby, R., Chvatal, V., 2006a. Concorde tsp solver http://www.math.uwaterloo.ca/tsp/concorde/index.html.
- Applegate, D., Bixby, R., Chvatal, V., Cook, W., 2006b. The traveling salesman problem: a computational study. Princeton University Press.
- Applegate, D., Cook, W., Rohe, A., 2003. Chained lin-kernighan for large traveling salesman problems. INFORMS Journal on Computing 15, 82–92.
- Bao, X., Liu, Z., 2012. An improved approximation algorithm for the clustered traveling salesman problem. Information Processing Letters 112, 908–910.
- Bao, X., Liu, Z., Yu, W., Li, G., 2017. A note on approximation algorithms of the clustered traveling salesman problem. Information Processing Letters 127, 54–57.
- Campuzano, G., Obreque, C., Aguayo, M.M., 2020. Accelerating the miller-tucker-zemlin model for the asymmetric traveling salesman problem. Expert Systems with Applications 148, 113229.
- Chisman, J.A., 1975. The clustered traveling salesman problem. Computers & Operations Research 2, 115–119.
- Claus, A., 1984. A new formulation for the travelling salesman problem. SIAM Journal on Algebraic Discrete Methods 5, 21–25.
- Cosma, O., Pop, P.C., Cosma, L., 2021. An effective hybrid genetic algorithm for solving the generalized traveling salesman problem. Lecture Notes in Computer Science 12886, 113–123.
- Ding, C., Cheng, Y., He, M., 2007. Two-level genetic algorithm for clustered traveling salesman problem with application in large-scale tsps. Tsinghua Science and Technology 12, 459–465.
- Dolan, E.D., Moré, J.J., 2002. Benchmarking optimization software with performance profiles. Mathematical Programming 91, 201–213.
- Dubois-Lacoste, J., Hoos, H.H., Stützle, T., 2015. On the empirical scaling behaviour of state-of-the-art local search algorithms for the euclidean tsp. In Proceedings of the 2015 Annual Conference on Genetic and Evolutionary Computation (pp. 377-384).
- Fischetti, M., Salazar González, J.J., Toth, P., 1997. A branch-and-cut algo-

- rithm for the symmetric generalized traveling salesman problem. Operations Research 45, 378–394.
- Gendreau, M., Laporte, G., Hertz, A., 1997. An approximation algorithm for the traveling salesman problem with backhauls. Operations Research 45, 639–641.
- Ghaziri, H., Osman, I.H., 2003. A neural network algorithm for the traveling salesman problem with backhauls. Computers & Industrial Engineering 44, 267–281.
- Guttmann-Beck, N., Hassin, R., Khuller, S., Raghavachari, B., 2000. Approximation algorithms with bounded performance guarantees for the clustered traveling salesman problem. Algorithmica 28, 422–437.
- Hà, M.H., Nguyen Phuong, H., Tran Ngoc Nhat, H., Langevin, A., Trépanier, M., 2022. Solving the clustered traveling salesman problem with-relaxed priority rule. International Transactions in Operational Research 29, 837–853.
- Hains, D., Whitley, D., Howe, A., 2012. Improving lin-kernighan-helsgaun with crossover on clustered instances of the tsp. In International Conference on Parallel Problem Solving from Nature (pp. 388-397). Springer, Berlin, Heidelberg.
- Helsgaun, K., 2000. An effective implementation of the lin-kernighan traveling salesman heuristic. European Journal of Operational Research 126, 106–130.
- Helsgaun, K., 2009. General k-opt submoves for the lin-kernighan tsp heuristic. Mathematical Programming Computation 1, 119–163.
- Helsgaun, K., 2014. Solving the clustered traveling salesman problem using the lin-kernighan-helsgaun algorithm. Computer Science Research Report (142), 1–45.
- Hoos, H.H., Stützle, T., 2014. On the empirical scaling of run-time for finding optimal solutions to the travelling salesman problem. European Journal of Operational Research 238, 87–94.
- Jin, Y., Hao, J.K., 2019. Solving the latin square completion problem by memetic graph coloring. IEEE Transactions on Evolutionary Computation 23, 1015–1028.
- Johnson, D.S., McGeoch, L.A., 2007. Experimental analysis of heuristics for the stsp. In The Traveling Salesman Problem and its Variations (pp. 369-443). Springer, Boston, HEA.
- Jongens, K., Volgenant, T., 1985. The symmetric clustered traveling salesman problem. European Journal of Operational Research 19, 68–75.
- Kawasaki, M., Takazawa, K., 2020. Improving approximation ratios for the clustered traveling salesman problem. Journal of the Operations Research Society of Japan 63, 60–70.
- Kerschke, P., Kotthoff, L., Bossek, J., Hoos, H.H., Trautmann, H., 2018. Leveraging tsp solver complementarity through machine learning. Evolutionary computation 26, 597–620.
- Kotthoff, L., Kerschke, P., Hoos, H., Trautmann, H., 2015. Improving the state of the art in inexact tsp solving using per-instance algorithm selection.

- In International Conference on Learning and Intelligent Optimization (pp. 202-217). Springer, Cham.
- Laporte, G., Palekar, U., 2002. Some applications of the clustered travelling salesman problem. Journal of the Operational Research Society 53, 972–976.
- Laporte, G., Potvin, J.Y., Quilleret, F., 1997. A tabu search heuristic using genetic diversification for the clustered traveling salesman problem. Journal of Heuristics 2, 187–200.
- Lin, S., Kernighan, B.W., 1973. An effective heuristic algorithm for the traveling-salesman problem. Operations Research 21, 498–516.
- Lokin, F.C.J., 1979. Procedures for travelling salesman problems with additional constraints. European Journal of Operational Research 3, 135–141.
- Martin, O., Otto, S.W., Felten, E.W., 1991. Large-step markov chains for the traveling salesman problem. Oregon Graduate Institute of Science and Technology, Department of Computer Science and Engineering.
- Mestria, M., 2016. A hybrid heuristic algorithm for the clustered traveling salesman problem. Pesquisa Operacional 36, 113–132.
- Mestria, M., 2018. New hybrid heuristic algorithm for the clustered traveling salesman problem. Computers & Industrial Engineering 116, 1–12.
- Mestria, M., Ochi, L.S., de Lima Martins, S., 2013. Grasp with path relinking for the symmetric euclidean clustered traveling salesman problem. Computers & Operations Research 40, 3218–3229.
- Miller, C.E., Tucker, A.W., Zemlin, R.A., 1960. Integer programming formulation of traveling salesman problems. Journal of the ACM 7, 326–329.
- Morán-Mirabal, L.F., Velarde, J.L.G., Resende, M.G.C., 2014. Randomized heuristics for the family traveling salesperson problem. International Transactions in Operational Research 21, 41–57.
- Nagata, Y., Kobayashi, S., 1997. Edge assembly crossover: A high-power genetic algorithm for the traveling salesman problem. 7th International Conference on Genetic Algorithms (pp. 450-457), Morgan Kaufmann, San Francisco.
- Nagata, Y., Kobayashi, S., 2013. A powerful genetic algorithm using edge assembly crossover for the traveling salesman problem. INFORMS Journal on Computing 25, 346–363.
- Nagata, Y., Soler, D., 2012. A new genetic algorithm for the asymmetric traveling salesman problem. Expert Systems with Applications 39, 8947–8953.
- Neto, D., 1999. Efficient cluster compensation for lin-kernighan heuristics. PhD thesis, University of Toronto .
- Pop, P., Matei, O., Pintea, C., 2018. A two-level diploid genetic based algorithm for solving the family traveling salesman problem, in: Proceedings of the Genetic and Evolutionary Computation Conference (pp. 340–346).
- Potvin, J.Y., Guertin, F., 1996. The clustered traveling salesman problem: A genetic approach. In Meta-Heuristics (pp. 619-631). Springer, Boston.
- Reinelt, G., 1991. Tsplib-a traveling salesman problem library. ORSA Journal on Computing 3, 376–384.

- Siqueira, A.S., da Silva, R.C., Santos, L.R., 2016. Perprof-py: A python package for performance profile of mathematical optimization software. Journal of Open Research Software, 4(1).
- Srivastava, S.S., Kumar, S., Garg, R.C., Sen, P., 1969. Generalized traveling salesman problem through n sets of nodes. CORS Journal 7, 97–101.
- Weintraub, A., Aboud, J., Fernandez, C., Laporte, G., Ramirez, E., 1999. An emergency vehicle dispatching system for an electric utility in chile. Journal of the Operational Research Society 50, 690–696.
- Wong, R., 1980. Integer programming formulations of the travelling salesman problem. Proceedings of the IEEE International Conference of Circuits and Computers (pp. 149-152).
- Wu, Q., Hao, J.K., 2015. Solving the winner determination problem via a weighted maximum clique heuristic. Expert Systems with Applications 42, 355–365.
- Zenklusen, R., 2019. A 1.5-approximation for path tsp, in: Proceedings of the Thirtieth Annual ACM-SIAM Symposium on Discrete Algorithms (pp. 1539-1549).