Appendix to New Exact Methods for Solving Quadratic Traveling Salesman Problem

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Bellman Equation for QTSP

We consider the following Bellman equation for QTSP.

$$\text{compute } V(N \setminus \{0\}, 0, 0, 0) \tag{1a}$$

$$V(U, i, j, f) = \begin{cases} \min_{k \in U} V(U \setminus \{k\}, 0, k, k) & \text{if } j = 0, \\ \min_{k \in U}(c_{ijk} + V(U \setminus \{k\}, j, k, f)) & \text{if } j \neq 0 \wedge U \neq \emptyset, \\ c_{j,0,f} + c_{i,j,0} & \text{if } j \neq 0 \wedge U = \emptyset. \end{cases} \tag{1b}$$

The Bellman equation has four state variables $\{U, i, j, f\}$ to represent QTSP: U is the set of unvisited customers, i is the previous customer visited, j is the current customer, and f is the first customer visited after 0. We assume all the tours start from location 0, eliminating symmetry without compromising generality. The first line of the equation (1b) defines $V(U, i, j, f)$ as the optimal cost of the tour that starts from 0 and visits all customers in U, when $j = 0$. The second and third line of the equation (1b) defines $V(U, i, j, f)$ as the optimal cost of the path $\langle i, j, \sigma_1, \ldots, \sigma_{|U|}, 0, f\rangle$, where $\{\sigma_1, \ldots, \sigma_{|U|}\} = U$. Equation (1a) defines the objective of the QTSP as the optimal cost of the tour that starts from 0 and visits all customers in $N \setminus \{0\}$. Observe that the target state in equation (1a) is the only state with $j = 0$, as j is assigned a customer in U in the recursive sub-problem formulation and U never contains customer 0.

Proof of the Bellman Equation for QTSP

In this section, we prove that the Bellman Equation (1a)-(1b) computes the smallest cost of any tour $\langle \sigma_1, \ldots, \sigma_n\rangle$ visiting all the customers in N.

The cost of a QTSP tour is defined as

$$C(\langle \sigma_1, \ldots, \sigma_n\rangle) = c_{\sigma_{n-1}\sigma_n\sigma_1} + c_{\sigma_n\sigma_1\sigma_2} + \sum_{i=1}^{n-2} c_{\sigma_i\sigma_{i+1}\sigma_{i+2}}. \tag{2}$$

In addition, we define cost of a QTSP path $\langle \sigma_1, ..., \sigma_k\rangle$ as

$$Q(\langle \sigma_1, ..., \sigma_k\rangle) = \sum_{i=1}^{k-2} c_{\sigma_i\sigma_{i+1}\sigma_{i+2}}. \tag{3}$$

Lemma 1. *If $U \subseteq N \setminus \{0\}$ and $j \neq 0$, then $V(U, i, j, f)$ in equation (1b) computes the cost of smallest path formed by an optimal sequencing σ^* of U, defined by $Q(\langle i, j, \sigma^*_1, ..., \sigma^*_{|U|}, 0, f\rangle)$, where $\{\sigma^*_1, ..., \sigma^*_{|U|}\} = U$.*

Proof. *We provide a proof by induction.*

Base Case: When $|U| = 0$ and $j \neq 0$, $V(U, i, j, f)$ is the cost of the only possible path $\langle i, j, 0, f\rangle$, and is thus the least-cost path, i.e., $V(U, i, j, f)$ takes the value in the third line (base case) of the Bellman equation (1b).

Inductive hypothesis: We assume that when $|U| = n$ and $j \neq 0$, $V(U, i, j, f)$ computes the smallest path cost $Q(\langle i, j, \sigma^*_1, ..., \sigma^*_{|U|}, 0, f\rangle)$ for a set $U \subseteq N \setminus \{0\}$.

Inductive Step: We prove that when $|U| = n + 1$ and $j \neq 0$, $V(U, i, j, f)$ *still* computes the smallest path cost $Q(\langle i, j, \sigma^*_1, ..., \sigma^*_{|U|}, 0, f\rangle)$, where $U \subseteq N \setminus \{0\}$.

From equation (1b), we know that when $n > 0$,

$$V(U, i, j, f) = \min_{k \in U}(c_{ijk} + V(U \setminus \{k\}, j, k, f)).$$

Since, $|U| = n + 1$, the cardinality of $U \setminus \{k\}$ must be n. Then, from the inductive hypothesis, we know that $\forall k \in U, V(U \setminus \{k\}, j, k, f))$ computes the smallest path cost $Q(\langle j, k, \sigma^*_1, ..., \sigma^*_{|U|-1}, 0, f\rangle)$, where $\{k, \sigma^*_1, ..., \sigma^*_{|U|-1}\} = U$.

Let $k^* = \arg\min_{k \in U}(c_{ijk^*} + V(U \setminus \{k^*\}, j, k^*, f))$. Then, for any path $\langle i, j, \sigma_1, ..., \sigma_{|U|}, 0, f\rangle$ with $\{\sigma_1, ..., \sigma_{|U|}\} = U$, it holds that

$$\begin{aligned} Q(\langle i, j, \sigma_1, ..., \sigma_U, 0, f\rangle) &= c_{ij\sigma_1} + Q(\langle j, \sigma_1, ..., \sigma_U, 0, f\rangle) \\ &\geq c_{ij\sigma_1} + V(U \setminus \{\sigma_1\}, j, \sigma_1, f) \\ &\geq c_{ijk^*} + V(U \setminus \{k^*\}, j, k^*, f) \\ &= V(U, i, j, f), \end{aligned}$$

proving that $V(U, i, j, f)$ computes the smallest path cost $Q(\langle i, j, \sigma^*_U, ..., \sigma^*_U, 0, f\rangle) \leq Q(\langle i, j, \sigma_1, ..., \sigma_U, 0, f\rangle)$ for all permutations σ with $\{\sigma_1, ..., \sigma_U\} = U$.

□

Theorem 2. *$V(N \setminus \{0\}, 0, 0, 0)$ computes the cost of an optimal tour $\langle 0, \sigma^*_1, \ldots, \sigma^*_{n-1}\rangle$ that visits all locations in N*

with the smallest cost, i.e., for all permulations σ of $N \setminus \{0\}$,

$$V(N \setminus \{0\}, 0, 0, 0) = C(\langle 0, \sigma_1^*, \ldots, \sigma_{|N|-1}^* \rangle) \\ \leq C(\langle 0, \sigma_1, \ldots, \sigma_{|N|-1} \rangle).$$

Note that we can fix the first visited customer to be 0, as the overall tour cost is invariant to this choice.

Proof. From Lemma 1, we know that $\forall k \in N \setminus \{0\}$, $V(N \setminus \{0, k\}, 0, k, k)$ is the smallest path cost $Q(\langle 0, k, \sigma_1'^*, ..., \sigma_{|N|-2}'^*, 0, k \rangle)$, where $\{\sigma_1'^*, ..., \sigma_{|N|-2}'^*\} = N \setminus \{0, k\}$.

Also, from equations (2) and (3), we know that the travel cost of a path $Q(\langle \sigma_1'', ..., \sigma_{|N|+2}'' \rangle)$ is the same as the tour cost $C(\langle \sigma_1'', \ldots, \sigma_{|N|}'' \rangle)$ when $\sigma_1'' = \sigma_{|N|+1}''$ and $\sigma_2'' = \sigma_{|N+2|}''$.

From the above and equation (1b), it follows that for all permutations σ of $N \setminus \{0\}$,

$$\begin{aligned} V(N \setminus \{0\}, 0, 0, 0) &= \min_{k \in N \setminus \{0\}} V(N \setminus \{0, k\}, 0, k, k) \\ &= V(N \setminus \{0, \sigma_1^*\}, 0, \sigma_1^*, \sigma_1^*) \\ &\leq V(N \setminus \{0, \sigma_1\}, 0, \sigma_1, \sigma_1) \\ &\leq Q(\langle 0, \sigma_1, \sigma_2, ..., \sigma_{|N|-1}, 0, \sigma_1 \rangle) \\ &= C(\langle 0, \sigma_1, \sigma_2, ..., \sigma_{|N|-1} \rangle), \end{aligned}$$

where $\sigma_1^* = \arg\min_{k \in N \setminus \{0\}} V(N \setminus \{0, k\}, 0, k, k)$. □

Additional Experiment Results

We include the performance graphs (Figure 1) with results from the CP-SAT solver on solving the two proposed CP models: CPSAT-AD, using an all-different constraint and CPSAT-CIR, with the circuit constraint. Both CP-SAT models trail their CP Optimizer counterparts in both primal gap and optimality gap measurements. Further, the CP-SAT approaches have a worse performance than all of the other exact approaches.

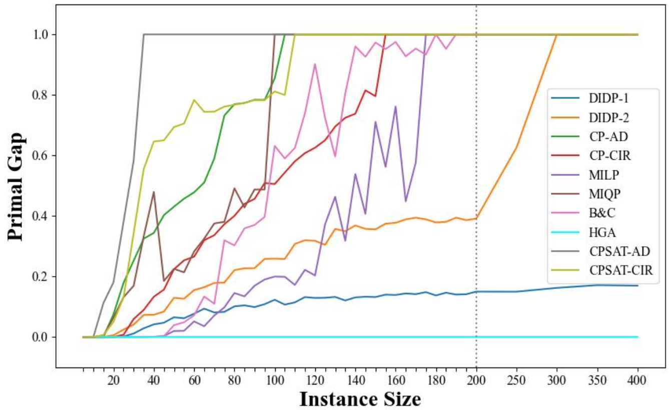
Diversity of Costs

To measure the difference between the minimum and the average traveling cost to each customer, we introduce the ratio between the mean and the minimum of all cost terms in each problem instance, i.e.,

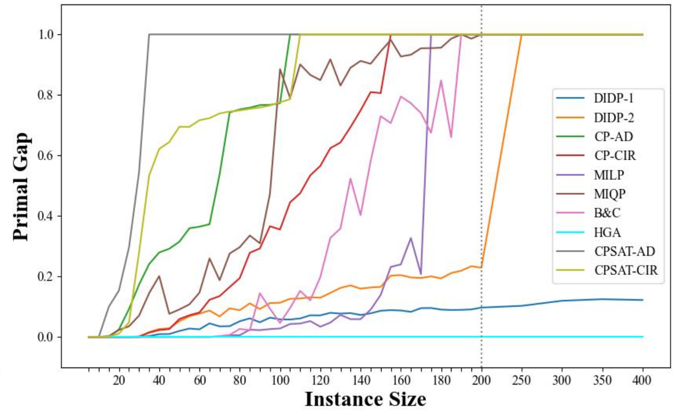
$$\frac{\text{mean}\{c_{ijk} | i, j, k \in N, i \neq j, j \neq k, i \neq k\}}{\min\{c_{ijk} | i, j, k \in N, i \neq j, j \neq k, i \neq k\}}.$$

Figure 2a and 2b show the relationship between the mean-to-min ratio of the costs and the optimality gap that each DIDP approach can achieve. The AngleDistance instances have a smaller mean-to-min ratio that correlates with the optimality gap that is achieved by the two DIDP models. The data points that have 0 optimality gap correspond to the instances with up to 10 customers, which are easy to solve regardless of the mean-to-min ratio.

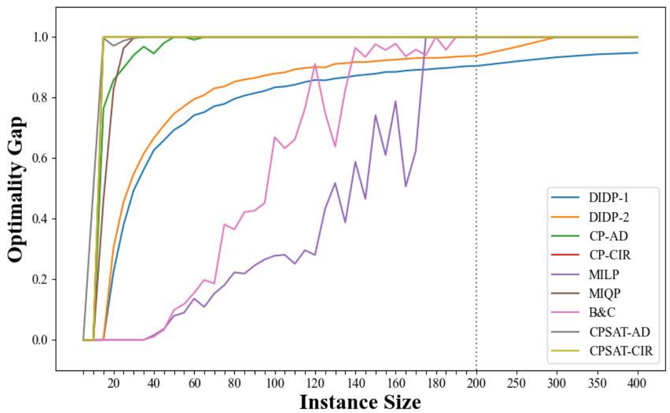
(a) Average *primal gap* for Angle-TSP instances.



(b) Average *primal gap* for AngleDistance-TSP instances.



(c) Average *optimality gap* for Angle-TSP instances.



(d) Average *optimality gap* for AngleDistance-TSP instances.

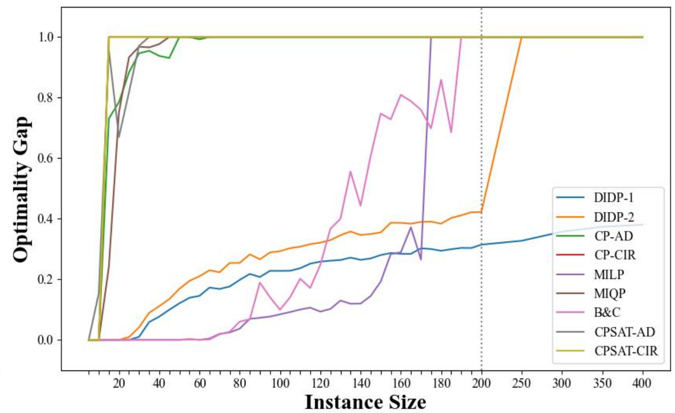
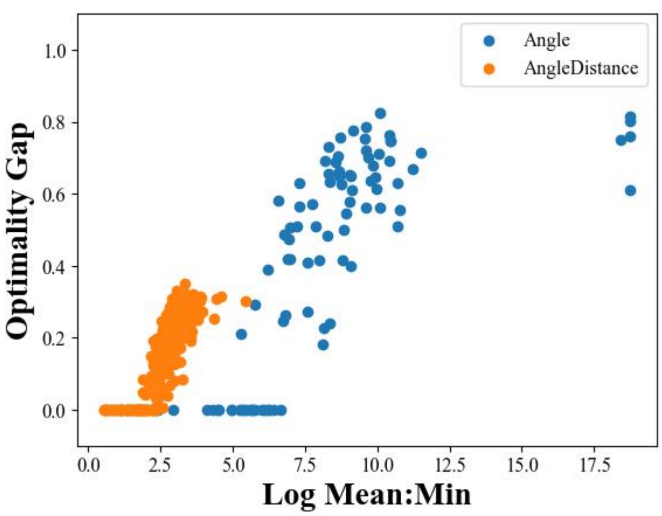


Figure 1: The plots of average *primal gap* and *optimality gap* found by each solver.

(a) The optimality gap found by DIDP-1 vs. logarithm of the mean-to-min ratio.



(b) The optimality gap found by DIDP-2 vs. logarithm of the mean-to-min ratio.

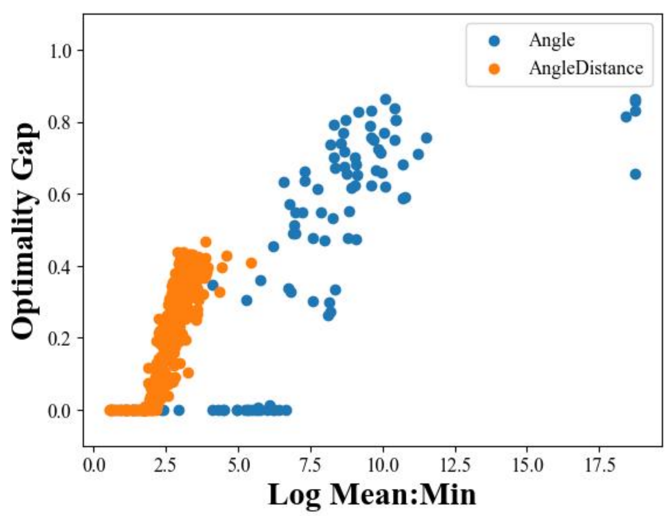


Figure 2: The relationship between the optimality gap found by the DIDP solvers and the ratio between the mean cost and the minimum cost in each instance.