A Massively Parallel Solver for QAPs

Official project title

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In Short

- The goal of the project is to solve previously unsolved challenging large scale Quadratic Assingment Problem (QAP) instances from QAPLIB.

For a positive integer n, we let $N = \{1, \ldots, n\}$ represent a set of locations and also a set of facilities. Given $n \times n$ symmetric matrices $\boldsymbol{A} = [a_{ik}]$, $\boldsymbol{B} = [b_{j\ell}]$ and an $n \times n$ matrix $\boldsymbol{C} = [c_{ij}]$, the quadratic assignment problem (QAP) is stated as

$$\min_{\pi} \sum_{i \in N}^{n} \sum_{k \in N}^{n} a_{ik} b_{\pi(i),\pi(k)} + \sum_{i \in N}^{n} c_{i,\pi(i)}, \tag{0.1}$$

where a_{ik} denotes the flow between facilities i and k, $b_{j\ell}$ is the distance between locations j and ℓ, c_{ij} the fixed cost of assigning facility i to location j, and $(\pi(1), \ldots, \pi(n))$ a permutation of $1, \ldots, n$ such that $\pi(i) = j$ if facility i is assigned to location j.

The QAP is one of the most renowned classical combinatorial optimization problems. The QAPLIB [3], first published in 1991, aimed to provide a unified testbed for the QAP that is widely accessible to the scientific community. It has been continuously updated to stimulate further research into this critical problem class. Consequently, the QAP has been extensively studied over the last three decades, both theoretically and computationally.

Solving QAP instances larger than size 35 remains a significant challenge in practice, despite the QAP being known as NP-hard theoretically. Various heuristic methods for the QAP, such as tabu search, genetic algorithms, and simulated annealing, have been developed. These methods frequently achieve near-optimal solutions, which often coincide with the exact optimal solutions. However, the exactness of these solutions is not guaranteed in general.

Most existing methods for finding the exact solutions of QAP are designed within the branch-and-bound (B&B) algorithmic framework [1,4]. As the name suggests, branching and lower bounding constitute the core procedures of this method.

Lower bounding procedures incorporated in the branch-and-bound method plays a crucial role. They have been developed for decades; Gilmore-Lawler bound, Reformulation-Linearization Technique, spectral methods, semidefinite programming (SDP) relaxations. To apply a strong lower bounding procedure, we employ the Lagrangian doubly nonnegative (DNN) relaxation and the Newton-bracketing method. Though, DNN relaxation is known to be stronger than SDP relaxation, its highly degenerate nature makes difficult to solve by well-known methods as primal-dual interior point methods.

First two of the methods are SDPNAL+ [12] (a majorized semismooth Newton-CG augmented Lagrangian method for semidefinite programming with nonnegative constraints) and BBCPOP [5] (a bisection and projection method for Binary, Box and Complementary constrained Polynomial Optimization Problems). Some numerical results on these two methods applied to DNN relaxation of QAP instances with dimensions $n = 15$ to 50 from QAPLIB were reported in [5], where BBCPOP attained tighter lower bounds for many of instances with dimensions 30 to 50 in less execution time. The third method is an alternating direction method of multipliers (ADMM) proposed by Oliveira et al. [7] in combination with facial reduction for robustness. The fourth method is the Newton-bracketing (NB) method [6], which was recently proposed to enhance the lower bounds. The NB method employs the Accelerated Proximal Gradient (APG) method internally, enabling stable solutions for large-scale DNN relaxation. It theoretically possesses the desirable property as quadratic convergence. New and improved lower bounds for the unknown minimum values of larger scale QAP instances, including tai100a and tai100b, were computed using the Newton-bracketing method; see QAPLIB [3].

To solve large scale QAPs, massive paralellization is crucial. We adapted UG, generic framework to parallelize branch-and-bound based solvers. It has achieved large-scale MPI parallelism with 80,000 cores [8]. We have integerated our QAP solver with UG to realize a large-scale, parallelized solver.

The main motivation of our project is to challenge larger scale QAP instances from QAPLIB [3] that have not been solved yet. We implement the NB method [6] combined with the B&B method in the specialized Ubiquity Generator (UG) framework [11] to find the exact solutions of large scale QAP instances. See Sections 2, 3, 4, 5 in [2] for precise and detailed description about the proposed algorithms.

We solved challenging large scale instances, nug30, tai30a, tai35b, tai40b and sko42 on the ISM (Institute of Statistical Mathematics) supercomputer HPE SGI 8600, which is a liquid cooled, tray-based, high-density clustered computer system. The ISM supercomputer has 384 computing nodes and each node has two Intel Xeon Gold 6154 3.0GHz CPUs (36 cores) and 384GB of memory. All of the instances were solved as a single job. Table 1 shows the computational results. Note that tai30a and sko42 were solved to the optimality for the first time, which had remained unsolved for more than 20 years.

Table 1: *Numerical results on challenging large scale QAP instances.*

QAP instance	Opt.val	No. of nodes generated	Total execution time(sec) in para.	No. of CPU cores used
nug30	6,124	26,181	3.14e3	1,728
tai30a	1,818,146	34,000,579	5.81e5	1,728
tai35b	283,315,445	2,620,547	2.49e5	1,728
tai40b	637,250,948	278,465	1.05e5	1,728
sko42	15,812	6,019,419	5.12e5	5,184

We address the recent advancements in solving tai50b, noting a significant increase in the lower bounds. With the current solution process, dedicating more time to the problem will likely reach to obtain the exact solution. Figure 1 shows the current solution process of tai50b. Our approach emphasizes the importance of continued efforts and resource allocation to fully exploit the potential for solving tai50b.

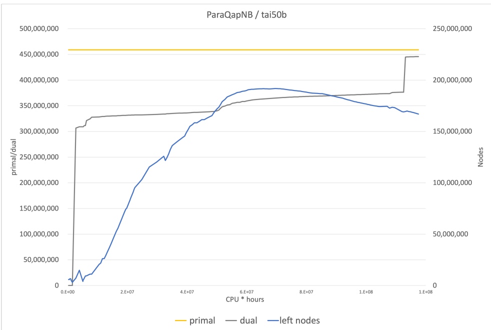

Figure 1: *solution process of tai50b*

The goal of this project is to (further) develop the parallel QAP solver based UG to handle over 100,000 cores to solve notoriously hard QAP instances to the optimality. We believe that this project would serve as a flagship for the efficient solution of $\mathcal{NP}$-hard combinatorial optimization problems by using supercomputers.

WWW

https://www.zib.de/members/shinano,
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More Information

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DFG Subject Area

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