An Efficient Implementation of the Robust Tabu Search Heuristic for Sparse Quadratic Assignment Problems

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Abstract

We propose and develop an efficient implementation of the robust tabu search heuristic for sparse quadratic assignment problems. The traditional implementation of the heuristic applicable to all quadratic assignment problems is of $O(N^2)$ complexity per iteration for problems of size $N$. Using multiple priority queues to determine the next best move instead of scanning all possible moves, and using adjacency lists to minimize the operations needed to determine the cost of moves, we reduce the asymptotic ($N \to \infty$) complexity per iteration to $O(N \log N)$. For practical sized problems, the complexity is $O(N)$.

Keywords: Combinatorial optimization, Computing science, Heuristics, Tabu search

1. Introduction

The quadratic assignment problem (QAP) is a combinatorial optimization problem first introduced by Koopmans and Beckman (1957). It is NP-hard and is considered to be one of the most difficult problems to be solved optimally. The problem was defined in the following context: A set of $N$ facilities are to be located at $N$ locations. The distance between locations $i$ and $j$ is $D_{i,j}$ and the quantity of materials which flow between facilities $i$ and $j$ is $F_{i,j}$. The problem is to assign to each location a single facility so as to minimize the cost

$$C = \sum_{i=1}^{N} \sum_{j=1}^{N} F_{i,j} D_{p(i),p(j)},$$

where $p(i)$ represents the location to which facility $i$ is assigned. It will be helpful to think of the $N$ facilities and the matrix of flows between them in graph theoretic terms as a graph of $N$ nodes and weighted edges, respectively.

There is an extensive literature which addresses the QAP and is reviewed in Pardalos et al. (1994), Cela (1998), Anstreicher (2003), Loiola et al. (2007, and James et al. (2009a). With the exception of specially constructed cases, optimal algorithms have solved only relatively small instances with $N \leq 36$. Various heuristic approaches have been developed and applied to problems typically of size $N \approx 100$ or less. One of the most successful heuristics to date for large instances is robust tabu search, RTS, (Taillard (1991). The use of tabu search for the quadratic assignment problem has been studied extensively (Drezner (2005), Hasegawa et al. (2000), James et al, (2009a, 2009b), McLoughlin and Cedeno (2005), Misevicius (2007), Misevicius and Ostreika (2007), Skorinkapov (1994), and Wang (2007)). Some of the best available algorithms for the solution of the QAP are the hybrid genetic algorithms that use tabu search as an improvement mechanism. (See Drezner (2008)).

Here we will consider the robust tabu heuristic applied to sparse QAP instances. That is, the number of non-zero entries in the either the flow matrix and/or the distance matrix is of $O(N)$ as opposed to $O(N^2)$. Without loss of generality we will assume the flow matrix is sparse. Many real world problems are sparse. In fact, this work was motivated by the study of random regular sparse graphs. These graphs are very robust to partitioning and collapse due to removal of nodes or edges. We are interested in the problem of determining how to assign the nodes of such a graph to locations in a metric space such that the total edge length of the graph is minimized; this problem maps directly to
a quadratic assignment problem.

There has been some previous work on sparse quadratic assignment problems. Milos and Magirou (1995) developed a Lagrangian-relaxation lower-bound algorithm for sparse problems and Panos et al. (1997) developed a version of their GRASP heuristic for sparse problems. However, to the best of our knowledge, an efficient implementation of the robust tabu heuristic for sparse QAP instances has not been proposed.

2. Background - the tabu heuristic

The tabu heuristic for the quadratic assignment problem consists of repeatedly swapping locations of two nodes. A single iteration of the heuristic consists of

(a) Determining the move which most decreases the total cost. Under certain conditions (see Section 4), if a move which lowers the cost is not available, a move which raises the cost is made. So that cycles of the same moves are avoided, the same move is forbidden (taboo) until a specified later iteration; we call this later iteration the **eligible iteration** for a given move. This eligible iteration is traditionally stored in a **tabu list** or **tabu table**.

(b) Making the move.

(c) Recalculating the new cost of all moves.

The process is repeated for a specified number of iterations. Traditional implementations of robust tabu search require \( O(N^2) \) operations per iteration. The complexity of \( O(N^2) \) is achieved by maintaining a matrix containing the cost \( \Delta(p, u, v) \) of swapping \( u \) and \( v \) for all \( u \) and \( v \), given a current assignment \( p \).

The complexity of the each step above is as follows:

(a) \( O(N^2) \) - all possible \( N(N - 1)/2 \) moves are considered. The cost of each move is retrieved from \( \Delta(p, r, s) \)

(b) \( O(1) \) - the locations of the two swapped nodes are simply transposed.

(c) \( O(N^2) \) - based on the following observations of Taillard (1991):

Following Taillard (1991), starting from an assignment of facilities \( p \) let the resulting assignment after swapping facilities \( r \) and \( s \) be \( p' \).

That is:

\[
\begin{align*}
p'(k) &= p(k) \quad k \neq r, s \\
p'(r) &= p(s) \\
p'(s) &= p(r).
\end{align*}
\]  

For a symmetrical matrix with a null-diagonal, the cost \( \Delta(p, r, s) \) of swapping \( r \) and \( s \) is:

\[
\Delta(p, r, s) = \sum_{i=1}^{N} \sum_{j=1}^{N} (F_{i,j}D_{p(i),p(j)} - F_{i,j}D'_{p'(i),p'(j)})
\]

\[
= 2 \sum_{k \neq r,s} (F_{s,k} - F_{r,k}) (D_{p(s),p(k)} - D_{p(r),p(s)})
\]

To calculate \( \Delta(p', u, v) \) for any \( u \) and \( v \) with complexity \( O(N) \), we can use equation xx. For asymmetric matrices or matrices with non-null diagonals, a slightly more complicated version of Equation xx is given by Burkhard and Rendl (1984).

To calculate \( \Delta(p', u, v) \) in the case that the swapped facilities \( u \) and \( v \) are different from \( r \) or \( s \), we use the value \( \Delta(p, u, v) \) calculated in the previous iteration and find:

\[
\Delta(p', u, v) = \Delta(p, u, v) + 2(F_{r,u} - F_{r,v} + F_{s,v} - F_{s,u})
\]

\[
\cdot(D_{p'(s),p'(u)} - D_{p'(s),p'(v)} + D_{p'(r),p'(v)} - D_{p'(r),p'(u)})
\]  

(i) the cost of moves which do not involve the two nodes in the previous move can be calculated in time \( O(1) \). There are \( O(N^2) \) of these moves.

(ii) The cost of moves which do involve the two nodes in the previous move must be calculated from scratch. There are \( O(N) \) of these moves and the complexity of calculating each is \( O(N) \).

3. Approach

To reduce the complexity of step (a), instead of scanning all possible moves, we use multiple **priority queues** (PQs) to determine the best move. A priority queue is a data structure for maintaining a set of elements each of which has an associated value (priority). A PQ supports the following operations:
• Insert an item
• Remove an item
• Return the item with the highest value

Priority queues are used to efficiently find an item with the highest value without searching through all of the items.

The maximum complexity of PQ operations is $O(\log N)$. We will see below that there will be $O(N)$ insertions and deletions in the PQs for each iteration so the asymptotic complexity of this step is reduced to $O(N \log N)$. Furthermore, we will show that for problems of any practical size, PQ operations are not the determinant of total complexity.

The complexity to recalculate the cost of moves in step (c), can be reduced to $O(N)$ as follows:

• As in the traditional robust tabu implementation, the cost of moves which do not involve the two nodes in the previous move can be calculated in time $O(1)$. On average, there are $2\langle k \rangle$ nodes which are connected to the two nodes in the previous moves, where $\langle k \rangle$ is the average degree (average number of nodes adjacent to a given node) of the graph corresponding to the flow matrix. For each of these $2\langle k \rangle$ nodes we must calculate the cost of $N - 1$ possible moves. Thus, the cost is $O(\langle k \rangle N)$.

• The cost of moves which do involve the two nodes in the previous move must be calculated from scratch. There are $O(N)$ of these moves and the complexity of calculating each is $O(\langle k \rangle)$ since the cost of a node, $u$, being in a specific location depends only on the on-average $k$ nodes adjacent to $u$.

Thus the complexity of step (c) is reduced to $O(N)$.

4. Implementation

To describe our implementation, we must first describe the rules for determining the next move of Taillard’s robust tabu heuristic (Taillard (1991)). The following definitions for the possible state of a potential move are useful:

(i) If the current iteration is less than or equal to the eligible iteration, the move is ineligible.

(ii) If the current iteration is greater than the eligible iteration, the move is authorized.

(iii) If the current iteration minus an aspiration constant is greater than the eligible iteration the move is aspired.

The rules for determining the next move can then be stated as (Taillard (1991)):

(1) If a move which decreases the lowest total cost found so far is available, the move which most decreases this total cost is chosen, independent of whether the move is ineligible, authorized or aspired.

(2) If no move meets criterion (1), the aspired move, if one is available, which most decreases the current total cost is chosen.

(3) If no moves meet criteria (1) or (2), the lowest cost authorized move is chosen.

To implement these rules for sparse problems, we use two types of PQs: delta PQs which contain the cost delta for a given move and tabu PQs which contain entries ordered by the eligible iteration for the move. The tabu PQs control the change of state of a move. The delta PQs determine the lowest cost move in each state. Five PQs are used:

• ineligible tabu PQ - This PQ contains moves, ordered by eligible iteration, which are in the ineligible state. This PQ allows us to efficiently determine when the state of a move can be changed to authorized.

• authorized tabu PQ - This PQ contains moves, ordered by eligible iteration, which are in the
authorized state. This PQ allows us to efficiently determine when the state of a move can be changed to aspired.

- ineligible delta PQ - This PQ contains moves, ordered by the cost of the move, which are in the ineligible state. This PQ together with the two other delta PQs allows for efficient determination of the overall lowest cost move as required by rule 1.

- aspired delta PQ - This PQ contains moves, ordered by the cost of the move, which are in the aspired state. This PQ allows for efficient determination of the lowest cost aspired move as required by rule 2.

- authorized delta PQ - This PQ contains moves, ordered by the cost of the move, which are in the authorized state. This PQ allows us to determine the lowest cost authorized move as needed by rule 3.

As illustrated in Fig. 1, moves are inserted and removed in the PQs under the following circumstances:

- At initialization all moves are inserted into the ineligible PQs.

- At the beginning of each iteration, any moves on the ineligible PQs which become authorized, because the iteration has increased by one, are moved from the ineligible PQs to the authorized PQs.

- At the beginning of each iteration, any moves on the authorized PQs which become aspired, because the iteration has increased by one, are moved to the aspired PQ.

- After each move, any move for which the move cost or eligible iteration has changed is removed from the PQ in which it is present and inserted in the appropriate PQ based on move state and move cost. (However, see lazy update discussion below.)

Using these PQs we obtain exactly the same results as the traditional robust tabu implementation.

5. Lazy Update

We minimize the time updating PQs by performing lazy updates. After a change in the eligible iteration or move cost, if the state is changed or the value is increased, we update the PQs involved; otherwise, we perform a lazy update and store the value in a data structure associated with the move and only do the update in the PQ when and if the move becomes the move with the smallest value in the PQ. This use of lazy updates significantly decreases the time spent on PQ operations.

![Figure 2: The ratio of the time per iteration for the non-sparse implementation to the time per iteration for the sparse implementation versus the problem size, $N$. The slope of the plot is approximately 1.0 which is consistent with a reduction of $O(N)$ of the computational complexity.](image)

Figure 3: The time per iteration for the non-sparse (upper plot) and sparse (lower plot) implementations.

6. Numerical Results

We test our algorithm on instances with $N$ locations on a square grid with a Euclidean metric. The flow matrix for the $N$ facilities corresponds to
an adjacency matrix for a $k$-regular random graph; that is, each facility has flows of value one to $k$ other random facilities. We run both the traditional non-sparse implementation and our new sparse implementation. The non-sparse implementation is the code of Taillard (1991). To implement the priority queues in the sparse implementation, we use the complete balanced tree code of Marin and Cordero (1995). We perform a minimum of $10^4$ iterations for each instance.

For $N = 2500$, priority queue update operations consume just 2% of the total time. Assuming a $\log{N}$ behavior for PQ operations, it is not until $N$ becomes astronomically large that the PQ operations would take the majority of the time and the behavior of our implementation crosses over from $O(N)$ to $O(N\log{N})$ complexity. We thus expect $O(N)$ complexity for our sparse implementation for any practical sized problems.

In Fig. 2 for $k = 3$, we plot the ratio $r$ of the time per iteration of the non-sparse implementation to the time per iteration of the sparse implementation versus $N$. As expected, the plot is consistent with $r \sim N^x$ where $x \approx 1.0$. This reflects the reduction in complexity from $O(N^2)$ to $O(N)$. In Fig. 3 we plot separately the time per iteration for the original and the sparse implementations. Consistent with Fig. 2, the slopes on the log-log plot differ by 1 but the slopes are 2.5 and 1.5, respectively, as opposed to the theoretical values of 2.0 and 1.0. As explained in Paul (2007) and Saavedra and Smith (1995), this is due to the finite size of processor cache memory; as the problem size (and memory needed) increases, there is a smaller percentage of cache hits causing slower operation.

In Fig. 4 we plot the time per iteration versus values of degree $k$. The plot is linear with a slight deviation with increasing $k$. This deviation from linear is due to the fact that as $k$ increases there is an increasing chance that a node $u$ will be connected to both nodes involved in the previous move; however, the updated costs of moving node $u$ must be calculated only once.

We also performed numerical experiments on a class of problems known in the literature (see Drezner et al. (2005)). These problems denoted as DRExx are sparse and are designed to be very difficult to solve with heuristics. We obtained results similar to those for described above; performance is $O(N)$.

7. Summary

For sparse quadratic assignment problems, we reduce the asymptotic complexity per iteration of robust tabu search to $O(N\log{N})$ from $O(N^2)$; for practical size problems, the complexity is reduced to $O(N)$. Central to achieving this reduction is the use of multiple priority queues and lazy updates to these queues. The code which implements our approach and test QAP instances used for this paper are available as supplementary material.

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References

Anstreicher, K., 2003. Recent advances in the solution of quadratic assignment problems. Mathematical Programming 97, 27-42.

Burkhard R. E. F. Rendl, 1984. A thermodynamically motivated simulation procedure for combinatorial optimization problems. EJOR 17, 169-174.

Cela E., 1998. The Quadratic Assignment Problem: Theory and Algorithms. Kluwer, Boston, MA.

Cormen, T.H., Leiserson, C. E., Rivest R.L., Stein C., 2009. Introduction to Algorithms. MIT Press.
Drezner, Z., 2002. Heuristic algorithms for the solution of the quadratic assignment problem. Journal of Applied Mathematics and Decision Sciences 6, 163-173.

Drezner, Z., 2003. A new genetic algorithm for the quadratic assignment problem. INFORMS Journal of Computing 15, 320-330.

Drezner, Z., 2005. Compounded genetic algorithms. Operations Research Letters 33, 475-480.

Drezner, T., Drezner, Z., 2006. Gender-specific genetic algorithms. INFOR 2006 44 117-126.

Drezner, Z., 2005. A distance based rule for removing population members in genetic algorithms. 4OR 3, 109-116.

Drezner, Z. Marcoulides G.A., 2006. Mapping the convergence of genetic algorithms. Advances in Decision Science 2006 Article ID 70240, 16 pages.

Drezner, Z., 2005. The extended concentric tabu for the quadratic assignment problem. European Journal of Operational Research 160, 416-422.

Drezner, Z., Hahn, P.M., Taillard É., D., 2005. Recent Advances for the quadratic assignment problem with special emphasis on instances that are difficult for meta-heuristic methods. Annals of Operations Research 139, 65-94.

Drezner, Z. 2008. Extensive experiments with hybrid genetic algorithms for the solution of the quadratic assignment problem. Computers and Operations Research, 35, 717-736.

Drezner Z. and Marcoulides G., 2009. On the Range of Tabu Tenure in Solving Quadratic Assignment Problems Recent Advances in Computing and Management Information Systems. In: Recent Advances in Computing and Management Information Systems, 157-169 , P. Petratsos and G. A. Marcoulides (Eds), ATINER.

Hasegawa, M., Ikekuchi,T., Aihara, K., 2000. Exponential and chaotic neuodynamical tabu searches for quadratic assignment problems. CONTROL AND CYBERNETICS 29, 773-788.

James, T., Rego, C., Glover, F., 2009a. Multistart Tabu Search and Diversification Strategies for the Quadratic Assignment Problem. IEEE Tran. on Systems, Man, and Cybernetics PART A: SYSTEMS AND HUMANS 39, 579-596.

James, T., Rego, C., Glover, F., 2009b. A cooperative parallel tabu search algorithm for the quadratic assignment problem. European Journal of Operational Research 195, 810-826.

Koopmans T., Beckmann, M., 1957. Assignment problems and the location of economic activities. Econometrica 25, 53-76.

Loiola,E.M., de Abreu, N.M.M., Boaventuro-Netto, P.O., Hahn, P., Querido, T., 2007. A survey for the quadratic assignment problem. European Journal of Operational Research 176, 657-690.

Marin, M., Cordero P., 2007. An empirical assessment of priority queues in event-driven molecular dynamics simulation, Computer Physics Communications 92, 214-224.

McLoughlin, J. F., Cedeno, W., 2005. The Enhanced Evolutionary Tabu Search and its application to the Quadratic Assignment Problem. GECCO 2005: Genetic and Evolutionary Computation Conference 1, 975-982.

Milis, I. Z., Magirou V. F., 1995. A Lagrangian-relaxation algorithm for sparse quadratic assignment problems. Operations Research Letters. 17, 69-76.

Misevicius, A., 2007. A tabu search algorithm for the quadratic assignment problem. Computational Optimization and Applications 30, 95-111.

Misevicius,A., Ostreika, A., 2007. Defining tabu tenure for the quadratic assignment problem. Information Technology and Control. 36, 341-347.

Pardalos, P.M., Rendl, F., Wolkowicz, H., 1994. The quadratic assignment problem: A survey and recent developments. In: Pardalos, P.M., Wolkowicz, H., (Eds.), Quadratic Assignment and Related Problems. DIMACS Series on Discrete Mathematics and Theoretical Computer Science 16, Amer. Math. Soc., Baltimore, MD. 1-42.

Pardalos, P. M., Pitsoulis, L. S., Resende, M. G. C., 1997. Algorithm 769: Fortran subroutines for approximate solution of sparse quadratic assignment problems using GRASP. ACM Transactions on Mathematical Software (TOMS) 23, 196-208.

Paul, G., 2007. A Complexity O(1) priority queue for event driven molecular dynamics simulations. Journal of Computational Physics 221, 615-625.

R.H. Saavedra, Smith, A.J., 1995. Measuring cache and TLB performance and their effects on benchmark run times. IEEE Transactions on Computers 44, 1223-1235.

Skorinkapov, J., 1994. Extensions of a tabu search
adaptation to the quadratic assignment problem. Computers and Operations Research 121, 855-865.

Taillard, E., 1991. Robust taboo search for the quadratic assignment problem. Parallel Computing 17, 443-455; code available at http://mistic.heig-vd.ch/taillard/codes.dir/tabouqap.cpp.

Wang, J. C., 2007. Solving Quadratic Assignment Problems by a Tabu Based Simulated Annealing Algorithm. ICIAS 2007: International Conference on Intelligent and Advanced Systems Proceedings, 75-80.