Improved Bounds for General QAPs via Semidefinite Relaxations

Hans D Mittelmann

School of Mathematical and Statistical Sciences
Arizona State University

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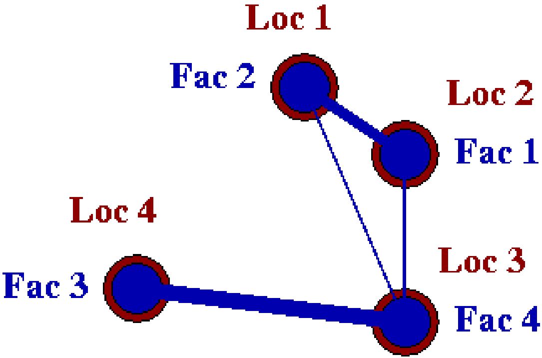
Outline

- Basic introduction
- A brief review
- New SDP relaxations of QAP
- New matrix splitting schemes
- Preliminary results
- Future direction

A QAP with four locations and facilities

Thickness of connections indicates level of flow



Optimal permutation: 2 1 4 3

A Mathematical Formulation of the Quadratic Assignment Problem

Mathematically, we can formulate the problem by defining two n by n matrices:

a *flow matrix* F whose (i,j) element represents the flow between facilities i and j,

and a *distance matrix* D whose (i,j) element represents the distance between locations i and j.

We represent an assignment by the vector p, which is a *permutation* of the numbers 1, 2, ... , n . p(j) is the location to which facility j is assigned.

With these definitions, the QAP can be written as

$$\min_{p \in \Pi} \sum_{i=1}^{n} \sum_{j=1}^{n} f_{ij} d_{p(i)p(j)}$$

Quadratic Assignment Problem (QAP)

$$\text{(QAP)} \qquad \min_{X \in \Pi} Tr(AXBX^T)$$

Π : the set of permutation matrices.

Both A and B are symmetric with nonnegative elements

- First introduced by Koopmans and Beckmann [1957]
- Many applications from various fields: facility location, communication…[QAPLib]
- Hundreds of papers dedicated to QAPs as listed in a recent survey by Hahn et al. [2007]

Existing approaches for QAPs

- Heuristics [Hahn et al. 07]
  - Genetic algorithm, tabu search, simulated annealing
- Exact methods
  - Branch&bound, cutting planes [Pardalos et al. 97, Brixius and Anstreicher 01, Hahn et al. 01,02]
  - Needs to solve some relaxed problem in the process to get a lower bound
  - The efficacy of the relaxation model plays a crucial role

Cheap Relaxations of QAPs

- Cheap relaxations that can be solved quickly
  - GLB reformulation [Gilmore 62 and Lawler 63],
  - QP relaxation [Anstreicher and Brixius 01],
  - Spectral bound based on eigenvalues and projection [Hadley-Rendl-Wolkowicz 92]
  - Weak bounds have been observed, especially when n becomes large
  - Resulting in a huge number of nodes in a B&B approach

Expensive QAP Relaxations

- LP relaxation based on ILP reformulation [Adams and Sherali 86, 90, Hahn et al. 98,01]
  - $z_{ijkl} = x_{ik} x_{jl}$ with extra constraints on z
- SDP relaxation based on matrix vectorization and Kronecker product [Zhao et al.98, Rendl et al.03]

Let $x = vector(X)$ *and* apply the standard SDP relaxation

to the matrix xx^T with extra constraints on the matrix elements.

- Tight bound but involves intensive computation
  - Out of the question for QAP instances of size n=50

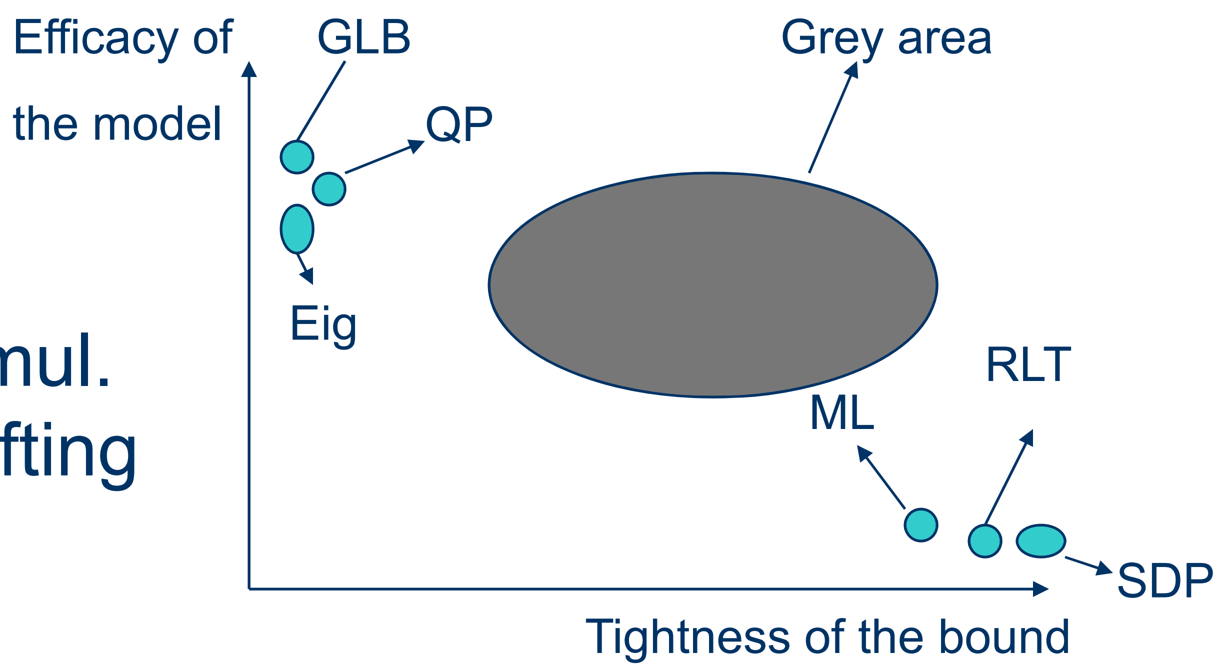
Resolution to the relaxation: I

- Improving algorithms for the expensive relaxations
  - Bundle methods [Rendl and Sotirov 03], exploring the symmetry [Klerk et al. 07], Lagrangian dual methods [Burer et al. 06, Hahn et al. 01]…
  - No reduction in the model's complexity,
    - The bottleneck, a large number of constraints and variables, still stands

Resolution to the relaxation: II

- Propose new relaxations that could be solved relatively easily and yet provide strong bounds
  - SDP relaxation based on matrix lifting [Ding and Wolkowicz, 06]
  - Relaxation over the cone of completely positive matrices [Povh and Rendl 06]
  - Many others such as QAP polytope…
  - Improvements over some expensive relaxations, but still not cheap

Efficacy VS Tightness



- RLT: reformul. based on lifting
- ML: matrix lifting

Motivation and Observation

- **Motivation:**
  - find cheap relaxations that yield strong bounds.
- **Observations:**
  - **Most relaxations are based on the binary structure of the matrix elements, not the algebraic feature of the permutation matrix itself!**
  - Specific QAPs arising from data mining have positive semidefinite matrices and large scale problems (n=1000s) have been solved based on SDP approaches

$$B \succ 0 \quad \Leftrightarrow \quad XBX^T \succ 0$$

Matrix Splitting

- **What to do when *B* is not PSD?**
  - Split the matrix into two parts OH,AH

$$B = B^+ - B^-, \quad B^+, B^- \succeq 0.$$

Both XB^+X^T **and** XB^-X^T **are positive semidefinite. Let** $Y^+ = XB^+X^T, Y^- = XB^-X^T$**, we have**

$$Y^+, Y^- \succeq 0.$$

New SDP relaxations

- Let e be the all 1 vector and *min(B)* the minimum element of B. Using the properties of X, we derive the following relaxation

$$
\begin{array}{lll}
\min & \mathbf{Tr}(A(Y^+ - Y^-)) & (1) \\
s.t. & Y^+ e = XB^+ e, \quad Y^- e = XB^- e; & \\
 & \mathbf{diag}(Y^+) = X\mathbf{diag}(B^+), \quad Y^+ \geq \min(B^+); & \\
 & \mathbf{diag}(Y^-) = X\mathbf{diag}(B^-), \quad Y^- \geq \min(B^-); & \\
 & Y^+ - XB^+X^T \succeq 0, \quad Y^- - XB^-X^T \succeq 0; & \\
 & Xe = X^T e = e, \quad X \geq 0. &
\end{array}
$$

One Theorem

- **Theorem:** The lower bound provided by the new SDP relaxation is always tighter than the bound derived by SDP relaxation based on matrix lifting in [Ding and Wolkowicz 06].
  - As observed in Ding-Wolkowicz paper, such a bound is comparable to the strongest SDP bounds.

Improvement and simplification

- We could swap A and B to derive a more complex SDP relaxation;
- Symmetries can be explored to improve the model;
- We could simplify the SDP constraints to

$$Y^+, Y^- \succeq 0.$$

  - Leading to certain speedup in the solving process, while without much loss of tightness of the bound

New Splitting Schemes: I

- **Definition:** We call the matrix splitting $B=B^{+}-B^{-}$ an orthogonal splitting if B^{+} and B^{-} are orthogonal to each other
  - Can be derived by using the singular value decomposition of B directly
  - Additional constraints can be added based on the orthogonality

New Splitting Schemes: II

- Suppose that B has only nonnegative elements. Let $d=Be$, and D be the diagonal matrix with diagonal elements d_i.
- Let $B=D-(D-B)$. $D-B$ refers to the so-called Laplace matrix in graph theory.
  - If B is associated with some graph, then many geometric properties of the Laplace matrix can be used to enhance the SDP relaxation

New Splitting Schemes: III

- Is it possible to get a splitting like $B=\alpha E-B^{-}$?
  - The problem can be addressed by solving an auxiliary SDP $\min_{\alpha E - B \succeq 0} \alpha.$
  - Two specific cases:
    - For QAPs from communication where B is the Hamming distance matrix of a hypercube in certain space, then such a dream splitting does exist, and α can be determined by the dimensionality of the hypercube!
    - For QAPs with matrices of Manhattan distance of rectangular grids, such a splitting is also easy to find

Preliminary Experiments

- **Computational environments:**
  - AMD Opteron with 2.4GHz CPU and 12 GB memory;
  - CVX, SDPT3 and Matlab 2007
  - Comparison to the models ($QAP_{L\text{-}S1}$, $QAP_{L\text{-}S2}$) in [Burer et al. 06] solved by the algorithm proposed in that paper, combined with commercial Cplex.

CVX script for basic model

```
e = ones(n,1);
E = e*e';
I = eye(n);
[V,D] = eig(B);
Dp = max(D, zeros(n));
Dm = max(Dp - D,zeros(n));
Bp = V*Dp*V';
Bm = V*Dm*V';
Dp = sqrtm(Dp);
Dm = sqrtm(Dm);
Rp = V*Dp;
Rm = V*Dm;
```

```
cvx_begin
    variable X(n,n)
    variable Yp(n,n) symmetric
    variable Ym(n,n) symmetric
    variable Zp(n,n)
    variable Zm(n,n)
    minimize( trace(A*(Yp-Ym)) )
    subject to
       diag(Yp) == X*diag(Bp);
       diag(Ym) == X*diag(Bm);
       Yp*e == X*Bp*e;
       Ym*e == X*Bm*e;
       tril(Yp,-1) - tril(Ym,-1) >= min(min(B));
       tril(Yp,-1) >= min(min(tril(Bp,-1)));
       tril(Ym,-1) >= min(min(tril(Bm,-1)));
```

```
%        norm(Yp + Ym,'fro') <= norm(B,'fro');
        Zp == X*Rp;
        Zm == X*Rm;
        lambda_min([I,Zp';Zp,Yp]) >= 0;
        lambda_min([I,Zm';Zm,Ym]) >= 0;
%        lambda_min(Yp) >= 0;
%        lambda_min(Ym) >= 0;
        X    >= 0;
        sum(X)  == 1;
        sum(X') == 1;
cvx_end
```

Numerical Results: I

Prob	$QAP_{L\text{-}S1}$	CPU	$QAP_{S\text{-}L2}$	CPU	Model-1	CPU
Nug25	18%	4665	3%	8914	11%	23s
Nug30	22%	11321	1%	26347	10%	72s
Tail30b	78%	12172	18%	50582	15%	161s
Tail35b	65%	24440	15%	141300	22%	322s
Tail40b	74%	43181	15%	330773	16%	763s

The relative gap is listed for comparison on tightness

Numerical Results: 2

Problem	Tail50b	Tail60b	Tail64C	Tail80b	Tail100b	Tail150b
New gap	18.4%	22.2%	2.4%	18.4%	22%	13.6%
Old gap	91.2%	91.8%	51.7%	89.1%	86.3%	87.4%

All the above problems have been solved within 40 minutes

Strong bounds have been obtained for QAPs of size up to n=256

From QAPLIB: E.D. Taillard [Taillard:91,Taillard:94]

name	n	feas.sol.		permutation/bound		gap
Tai40b	40	637250948	(Ro-TS)	544404685	(SDRMS)	14.57 %
Tai50a	50	4938796	(ITS)	4390920	(L&P)	11.09 %
Tai50b	50	458821517	(Ro-TS)	381474057	(SDRMS)	16.86 %
Tai60a	60	7205962	(TS-2)	5555095	(GLB)	22.91 %
Tai60b	60	608215054	(Ro-TS)	494776302	(SDRMS)	18.65 %
Tai64c	64	1855928	(Ro-TS)	1812779	(SDRMS)	2.32 %
Tai80a	80	13515450	(ITS)	10329674	(GLB)	23.57 %
Tai80b	80	818415043	(Ro-TS)	683526345	(SDRMS)	16.48 %
Tai100a	100	21052466	(ITS)	15824355	(GLB)	24.86 %
Tai100b	100	1185996137	(Ro-TS)	961844607	(SDRMS)	18.90 %
Tai150b	150	498896643	(GEN-3)	435738380	(SDRMS)	12.66 %
Tai256c	256	44759294	(ANT)	43849646	(SDRMS)	2.03 %

Conclusions

- New SDP relaxations based on various matrix splitting schemes;
- Much simpler than existing expensive relaxations, yet still provide strong bound;
- Allowing quick add-in or drop-off of constraints depending on the data structure;
- Can be easily embedded into the B&B approach;
  - A trial version of the B&B has been coded, and substantial improvement has been observed, though a long way is still ahead…..

Future Direction

- Exploring sparsity and symmetries in the data to enhance these new models;
- Develop Bender-type decomposition method for large scale QAP instances
- Design a rounding procedure to recover a feasible permutation and estimate the solution quality
- Investigate new branching rules to speed-up the B&B process…

References

- [1] H. Mittelmann and J. Peng. ***New Semidefinite Programming Relaxations for Quadratic Assignment Problems based on Matrix Splitting. In preparation.***
- [2] H. Mittelmann and J. Peng: ***Estimating Bounds for Quadratic Assignment Problems Associated with Hamming and Manhattan Distance Matrices based on Semidefinite Programming. Submitted to MP.***
- [3] S. Burer and D. Vandenbussche. **Solving lift-and-project relaxations of binary integer programs. SIAM Journal on Optimization 16, 726-750, 2006.**
- [4] Y. Ding and H. Wolkowicz. ***A matrix-lifting semidefinite relaxation for the quadratic assignment problem. Technical report CORR 06-22, University of Waterloo, Ontario, Canada, October,2006.***
- ***And many more ……***