Semidefinite and orthogonal relaxations: the QAP

Franz Rendl

http://www.math.uni-klu.ac.at

Alpen-Adria-Universität Klagenfurt

Austria

Overview

- Quadratic Assignment Problem
- Orthogonal Relaxations and Hoffman-Wielandt theorem
- Lagrangian duality and Anstreicher-Wolkowicz theorem
- SOS, SDP and copositive relaxations

The Quadratic Assignment Problem

Data: A, B symmetric matrices of order n
C: $n \times n$
(Π is set of permutation matrices)

$$\min_{X \in \Pi} \sum_{i,j,k,l} a_{i,j} b_{k,l} x_{i,k} x_{j,l} + \sum_{i,k} c_{i,k} x_{i,k}$$

More compact using the trace

$$\min_{X \in \Pi} \text{tr } AXBX^T + \text{tr } CX^T$$

QAP is NP-hard
Problems of size $n = 30$ considered very difficult

introduced by Koopmans, Beckmann (1957)

QAP: A small example

$$\text{tr } A(XBX^T)$$

Note that XBX^T is permuted B (after row/column permutation):

$$B = \begin{pmatrix} 1 & 7 & 0 & 1 \\ 7 & 2 & 6 & 8 \\ 0 & 6 & 3 & 9 \\ 1 & 8 & 9 & 4 \end{pmatrix}, \quad \pi = (3,1,4,2), \; X = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix},$$

$$XBX^T = \begin{pmatrix} 3 & 0 & 9 & 6 \\ 0 & 1 & 1 & 7 \\ 9 & 1 & 4 & 8 \\ 6 & 7 & 8 & 2 \end{pmatrix}$$

QAP: Related Problems

Traveling Salesman Problem
A is matrix of edge weights, B is adjacency matrix of tour

Bandwidth
A adjacency matrix, $b_{ij} = 1$ for $|i - j| > k$, else $b_{ij} = 0$
If value of QAP = 0, then bandwidth of A no more than k

Graph isomorphism
A, B adjacency matrices of two graphs G_A and G_B; these are isomorph iff $\exists X \in \Pi$ such that $A = XBX^T$, leads to QAP.

Complexity status unknown, but conjectured to be on the boundary between polynomial and NP-complete problems

QAP: Applications

- Location theory
- Wiring problems
- Hospital layout
- Graph theoretic problems (TSP, etc)

see e.g. E. Cela: QAP: Theory and Applications, Kluwer (1998)

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Orthogonal relaxations

Permutation matrices X are orthogonal.

What can we say about

$$\min_{X^TX=XX^T=I} \text{ tr } AXBX^T \text{ ??}$$

Notation: λ_A denotes vector of eigenvalues of (sym) A
$\lambda_A^+, (\lambda_A^-)$ vector sorted increasingly (decreasingly)

Hoffman-Wielandt Theorem:

$$\min_{X^TX=XX^T=I} \text{tr} AXBX^T = \langle \lambda_A^-, \lambda_B^+ \rangle$$

goes back to Hoffman, Wielandt (1957), J.v. Neumann (1937)

Orthogonal relaxation (2)

Permutation matrices also have row/column sums = 1.
Let V be $n \times (n-1)$ such that $V^T e = 0,\ V^T V = I_{n-1}$.

Parametrization

$$Xe = X^T e = e \text{ iff } \exists Y \text{ such that } X = \frac{1}{n} J + VYV^T$$

X orthogonal iff Y orthogonal

Substitute this into Hoffman-Wielandt Theorem to get better relaxation.

$$\text{tr} A(\frac{1}{n} J + VYV^T) B(\frac{1}{n} J + VY^T V^T) =$$

$$= \ldots = \text{tr}(V^T AV) Y (V^T BV) Y^T + \text{rest}$$

Orthogonal relaxation (3)

The quadratic part can be bounded using the Hoffman-Wielandt inequality.

The remaining part can be bounded independently by solving linear assignment problem.
This gives Projection bound from Hadley, Rendl, Wolkowicz, Math of OR (1992)

This will be shown to be equivalent to a special SDP bound.

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QAP: Lagrangian dual (1)

Alternative idea: Lagrangian dual

$$\min_{X^TX=XX^T=I} \text{tr } AXBX^T \geq$$

$$\max_{S,T} \min_{X} \text{ tr } [AXBX^T + S(I - XX^T) + T(I - X^TX)]$$

Here the Kronecker notation is useful: $x = vec(X)$, and

$$vec(AXB^T) = (B \otimes A)x$$

Cost function now $x^T(B \otimes A - I \otimes S - T \otimes I)x + \text{tr}(S + T)$.
The inner minimization is bounded only if

$$B \otimes A - I \otimes S - T \otimes I \succeq 0$$

QAP: Lagrangian dual (2)

Making this constraint explicit gives SDP:

$$\max_{S,T} \text{ tr } (S+T) \text{ such that } B \otimes A - I \otimes S - T \otimes I \succeq 0$$

How does it compare to the eigenvalue bound?

It's all the same: Theorem (Anstreicher, Wolkowicz (2001))
Orthogonal relaxation: $\min_{XX^T=X^TX=I}$ tr $AXBX^T =$
Lagrangian dual
$\max_{S,T}$ tr$(S+T):\ B \otimes A - I \otimes S - T \otimes I \succeq 0$

Note: SDP constraint is on matrix of order n^2.

Orthogonal relaxation involves eigenvalue decomposition of matrices of order n.

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QAP: Sum of Squares (SOS) Idea

Let us consider the function
$f(X) = \text{tr}\ [AXBX^T\ +\ S(I - XX^T)\ +\ T(I - X^TX)] + \sum_{ij} y_{ij}(x_{ij}^2 - x_{ij}) - \gamma.$
Here S, T, y and γ can be chosen arbitrarily.
If $f(X)$ is SOS, then we know that for any $X \in \Pi$

$$\text{tr}\ AXBX^T \geq \gamma$$

Best choice is given by $\max \gamma$ such that $f(X)\ SOS$.
Here the maximization is over S, T, y, γ. This leads again to SDP, in fact to the dual of SDP from before.
Prove this as exercise. (Hint: use Zhao et al. JOCO (1998))
Research Project:

Check stronger functions (with fourth order terms)

QAP: linearization idea

(QAP) $\min\langle AXB + C, X\rangle$ such that X is permutation matrix

Using $x =$ vec$(X), \; x \circ x = x$ we get

$$\langle AXB + C, X\rangle = \langle B \otimes A + \text{Diag}(vec(C)), xx^T\rangle$$

Now linearize $Y = xx^T$ to get SDP or copositive relaxations.

A technical problem:
How translate permutation properties from x to Y?

$$X = (x_1, \ldots, x_n), Y = \begin{pmatrix} Y^{11} & \ldots & Y^{1n} \\ \vdots & & \vdots \\ Y^{n1} & \ldots & Y^{nn} \end{pmatrix}, Y^{ij} = x_i x_j^T$$

QAP: linearization idea (2)

$$\sum_i Y^{ii} = \sum_i x_i x_i^T = I, \quad \text{tr}(Y^{ij}) = x_i^T x_j = \delta_{ij}$$

$$\langle J, Y \rangle = (e^T x)(x^T e) = n^2$$

X is orthogonal, sum of all elements is =n.

$$\mathcal{F} := \{Y \in C^*, \ \sum_i Y^{ii} = I, \ \text{tr}(Y^{ij}) = \delta_{ij}, \langle J, Y \rangle = n^2, \ \forall i, j\}$$

Theorem (J. Povh, F. Rendl 2005)

$\mathcal{F} = conv\{xx^T : x = vec(X), X$ permutation matrix$\} = \Pi$

Proof

By construction, $\Pi \subseteq \mathcal{F}$. Now let $Y \in \mathcal{F}$, hence
$Y = \sum_k y_k y_k^T = \sum_k Z_k$ and $y_k \geq 0$.
Y_k is $n \times n$ matrix formed from $y_k \in \mathbb{R}^{n^2}$.
The proof is based on the following facts:
(a) each main diagonal block Z_k^{ii} is diagonal
(b) each off diagonal block has diag$(Z_k^{ij}) = 0 \;\; \forall i \neq j$
(c) each Y_k has at most one nonzero in each row / column.
(d) Each Y_k is multiple of permutation matrix.

Copositive relaxation of QAP

$$L := B \otimes A + \text{Diag}(vec(C)).$$

As a consequence, QAP is equivalent to the copositive program

$$\min \langle L, Y \rangle \text{ such that}$$

$$\sum_i Y^{ii} = I, \;\; \text{tr}(Y^{ij}) = \delta_{ij}, \; \langle J, Y \rangle = n^2, \; Y \in C^*.$$

Replacing $Y \in C^*$ by $Y \succeq 0$ gives SDP relaxation investigated by Zhao, Karisch, Wolkowicz, Sotirov, Rendl. Further constraints could be added, like

$$Y_{ij,ik} = 0, \;\; Y \geq 0.$$

This leads to primal form of SDP presented before.