Solving QAP Using Bundle Methods

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Preliminaries

- $\mathcal{S}_k$ …space of $k \times k$ symmetric matrices
- $\mathrm{tr}(A)$ …trace of square matrix A
- $\mathrm{diag}(M)$ …vector of diagonal elements of M
- $\mathrm{Diag}(x)$ …adjoint of diag
- $A \otimes B$ …Kronecker product
- $A \circ B$ …Hadamard product
- Π …set of $n \times n$ permutation matrices

Quadratic Assignment Problem (QAP)

$$\begin{aligned} \mathrm{QAP}(A,B,C): \ \min \quad & \mathrm{tr}(AXB+C)X^T \\ \mathrm{s.\,t.} \quad & X \in \Pi \end{aligned}$$

- $A, B, C \in \mathbb{R}^{n \times n}, \quad A = A^T, B = B^T$

Semidefinite Relaxation of QAP

$$x = \mathrm{vec}(X) \;\hookrightarrow\; \mathcal{S}_{n^2+1}$$

The direct approach to SDP relaxation

- objective function for QAP:

$$q(X) = \mathrm{tr}\ L_Q Y_X$$

where

$$L_Q = \begin{bmatrix} 0 & \frac{1}{2}\,c^T \\ \frac{1}{2}\,c^T & B \otimes A \end{bmatrix} \qquad Y_X = \begin{bmatrix} 1 & x^T \\ x & xx^T \end{bmatrix}$$

$$x = \mathrm{vec}(X) \;\text{ and }\; c = \mathrm{vec}(C)$$

- constraint:

$$X_{ij}^2 - X_{ij} = 0 \Leftrightarrow \mathrm{diag}(Y_X) = \text{first row}(Y_X)$$

Lagrangian Relaxation

- SDP relaxation $\Leftrightarrow$ Lagrangian relaxation for appropriately constrained problem

- formulation of QAP

$$(\mathrm{QAP}_1) \qquad \begin{array}{rl} \mu_1 = \min & \mathrm{tr}\,(AXB+C)X^T \\ \text{s.t.} & X_{ij}^2 - X_{ij} = 0, \quad \forall i,j \end{array}$$

- lower bound:

$$\mu_r = \max_{\bar{w}} \ \min_{y} \left\{ y^T [L_Q + \mathrm{Arrow}(\bar{w})] y - w_0 \right\}$$

where

$$\mathrm{Arrow}(w) = \begin{bmatrix} w_0 & -\frac{1}{2} w^T \\ -\frac{1}{2} w & Diag(w) \end{bmatrix}$$

$$y^T = (x_0, x^T) \qquad \bar{w}^T = (w_0, w^T)$$

- we rewrite μ_r as

$$(\mathrm{D}_1) \qquad \mathbf{max} \quad -w_0$$
$$\text{s.t.} \qquad L_Q + \mathrm{Arrow}(\bar{w}) \succeq 0$$

- Lagrangian dual of (D_1)

$$(\mathrm{SDP}_1) \qquad \mathbf{min} \quad \mathrm{tr} \ L_Q Y$$
$$\text{s.t.} \qquad \mathrm{arrow}(Y) = e_0, \ Y \succeq 0$$

where

$$\mathrm{arrow}(Y) = \mathrm{diag}(Y) - (0, (Y_{0,1:n^2})^T)$$

Geometry of Relaxation

- $\mathcal{F}$ . . . feasible set of semidefinite relaxation (SDP_1)

- $$Y_X = \begin{bmatrix} 1 \\ \mathrm{vec}(X) \end{bmatrix} \begin{bmatrix} 1 & \mathrm{vec}(X)^T \end{bmatrix}, \quad X \in \Pi$$

  Y_X . . . rank–one matrices
  . . . extreme points of $\mathcal{F}$

- $\bar{\Pi} = \{Y_X, \quad x = \mathrm{vec}(X),\ X \in \Pi\}$

- barycenter of $\operatorname{conv}(\bar{\Pi})$:

$$\bar{Y} = \frac{1}{n!} \sum_{X \in \Pi} Y_X = \begin{bmatrix} 1 & \frac{1}{n!} e^T \\ \frac{1}{n!} e & D \end{bmatrix}$$

where

$$D = [\frac{1}{n^2} E \otimes E] + [\frac{1}{n^2(n-1)} (nI - E) \otimes (nI - E)]$$

– rank $(\bar{Y}) = (n-1)^2 + 1$
– $\mathcal{R}(\bar{Y}) = \mathcal{R}(\bar{V})$

where

$$\bar{V} = \begin{bmatrix} 1 & 0 \\ \frac{1}{n}(e \otimes e) & V \otimes V \end{bmatrix} \qquad V = \begin{bmatrix} I_{n-1} \\ -e_{n-1}^T \end{bmatrix}$$

- **minimal face:** $\quad \bar{V} \mathcal{S}_{(n-1)^2+1} \bar{V}^T$

$$
(\mathrm{SDP}_1) \qquad \begin{array}{ll} \min & \mathrm{tr}\ L_Q Y \\ \text{s.t.} & \mathrm{arrow}(Y) = e_0, \quad Y \succeq 0 \end{array}
$$

The projected problem

$$
(\mathrm{QAP}_2) \qquad \begin{array}{ll} \min & \mathrm{tr}\ (LR) \\ \text{s. t.} & \mathrm{arrow}(\bar{V} R \bar{V}^T) = e_0, \quad R \succeq 0 \end{array}
$$

where $\quad R \in \mathcal{S}_{(n-1)^2+1}, \quad L = V^T L_Q V$

Inequality Constraints

$$
(\mathrm{QAP}_3) \qquad \begin{array}{ll} \min & \mathrm{tr}\ (LR) \\ \text{s. t.} & \mathrm{arrow}(\bar{V} R \bar{V}^T) = e_0, \quad R \succeq 0 \\ & \bar{V} R \bar{V}^T \geq 0 \end{array}
$$

Bundle Method

$$
\text{(P)} \qquad \begin{array}{ll} \max & c(x) \\ \text{s. t.} & x \in X \ldots \text{"nice constraints"} \\ & Ax \leq b \ldots \text{"hard constraints"} \end{array}
$$

$c : \mathbb{R}^n \to \mathbb{R}$ ... concave function
X ... convex set of "nice structure"
$A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$
$Ax \leq b$ ... combinatorial constraints

- transformation of (QAP_3) into (P)

$$
\begin{array}{ll} \max & -\text{tr}\,(LR) \\ \text{s. t.} & \left.\begin{array}{l} \text{arrow}(\bar{V}R\bar{V}^T) = e_0 \\ R \succeq 0 \end{array}\right\} \ldots \text{"nice"} \\ & \bar{V}R\bar{V}^T \geq 0 \qquad\qquad \ldots \text{"hard"} \end{array}
$$

Solving the System QAP_2

we use *primal–dual interior–point* algorithm

- **primal problem**

$$
\begin{array}{lll}
(\mathrm{P}_2) & \min & \mathrm{tr}\,(LR) \\
& \text{s.t.} & \mathrm{arrow}(\bar{V} R \bar{V}^T) - e_0 = 0 \\
& & R \succeq 0
\end{array}
$$

- **dual problem**

$$
\begin{array}{lll}
(\mathrm{D}_2) & \max & -w_0 \\
& \text{s.t.} & L + \bar{V}^T \mathrm{Arrow}(\bar{w}) \bar{V} - Z = 0 \\
& & Z \succeq 0
\end{array}
$$

Z … dual slack variable

- **log–barrier problem** for D_2:

$$
\begin{array}{ll}
\min & \{-w_0 - \mu \log \det Z\} \\
\text{s.t.} & L + \bar{V}^T \mathrm{Arrow}(\bar{w}) \bar{V} + Z = 0 \\
& Z \succeq 0
\end{array}
$$

$\mu \in \mathbb{R}$ … barrier parameter

- **optimality conditions**:

$$
\begin{array}{lll}
\text{(KKT)} & F_p & := \operatorname{arrow}(\bar{V} R \bar{V}^T) - e_0 & = 0 \\
& F_d & := L + \bar{V}^T \operatorname{Arrow}(\bar{w}) \bar{V} - Z & = 0 \\
& F_{ZR} & := ZR - \mu I & = 0
\end{array}
$$

- **linearization for a search direction**:

$$
\begin{array}{lrcl}
(\delta\text{KKT}) & \operatorname{arrow}(\bar{V}(\delta R)\bar{V}^T) & = & -F_p \\
& \bar{V}^T \operatorname{Arrow}(\delta w) \bar{V} - \delta Z & = & -F_d \\
& (\delta Z) R + Z(\delta R) & = & -F_{ZR}
\end{array}
$$

- **final system**

$$
\begin{aligned}
& \operatorname{arrow}(\bar{V} Z^{-1} \bar{V}^T \operatorname{Arrow}(\delta w) \bar{V} R \bar{V}^T) \\
& \qquad = \mu \operatorname{arrow}(\bar{V} Z^{-1} \bar{V}^T) - e_0
\end{aligned}
$$

Table 1. QAPLIB instances

	Sol.	GLB	$*$	bundle
Nug12	578	493	547	555
Nug14	1014	852	967	993
Nug15	1150	963	1075	1116
Nug16a	1610	1314	1520	1581
Nug16b	1240	1022	1132	1190
Nug17	1732	1388	1604	1679
Nug18	1930	1554	1776	1845
Nug20	2570	2057	2326	2470
Nug21	2438	1833	2157	2339
Nug22	3596	2483	3234	3436
Had12	1652	1536	1648	1648
Had14	2724	2492	2703	2719
Had16	3720	3358	3648	3707
Had18	5358	4776	5226	5329
Had20	6922	6166	6758	6769

$*$ Q. Zhao, S. E. Karisch, F. Rendl, H. Wolkowicz, *Semidefinite Programming Relaxations for the Quadratic Assignment Problem*, Journal of Combinatorial Optimization 2, 71–109(1998)

TABLE 1. QAPLIB instances

	Sol.	GLB	*	bundle	no sym.
Nug12	578	493	547	555	558
Nug14	1014	852	967	993	
Nug15	1150	963	1075	1116	1118
Nug16a	1610	1314	1520	1581	
Nug16b	1240	1022	1132	1190	
Nug17	1732	1388	1604	1679	
Nug18	1930	1554	1776	1845	
Nug20	2570	2057	2326	2470	
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$$
\begin{aligned}
\min\ & \operatorname{tr}\,(LR) \\
& \operatorname{arrow}(\bar{V}R\bar{V}^T) = e_0,\ \bar{V}R\bar{V}^T \geq 0 \\
& b^0\operatorname{diag}(\bar{V}R\bar{V}^T) = I,\ o^0\operatorname{diag}(\bar{V}R\bar{V}^T) = I \\
& \mathcal{G}_J(\bar{V}R\bar{V}^T) \leq 0, \qquad R \succeq 0
\end{aligned}
$$

b^0diag …sum of diag. blocks equals identity

o^0diag …trace of each diag. block is 1 and
trace of off–diag. blocks is 0

$\mathcal{G}_J : \mathcal{S}_{n^2+1} \to \mathcal{S}_{n^2+1}$ … *Gangster operator*:

$$
(\mathcal{G}_J(Y))_{ij} := \begin{cases} Y_{ij} & \text{if } \ (i,j) \in J \\ 0 & \text{otherwise} \end{cases}
$$

Table 2. number of iterations (it)

inst.	Nug12	Nug14	Nug15	Nug16a	Nug16b	Nug17	Nug18
it	389	464	459	473	439	476	472
inst.	Nug20	Nug21	Nug22	Had12	Had14	Had16	Had18
it	684	620	476	386	545	999	528

Table 3. duration time for one function evaluation

n	12	14	15	16	17	18	20	21	22
time (sec)	8	22	30	54	79	104	222	280	373