A Restricted Dual Peaceman-Rachford Splitting Method for a Strengthened DNN Relaxation for QAP

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At: Modern Techniques of Very Large Scale Optimization

joint with: Naomi Graham, Hao Hu, Jiyoung Im, Xinxin Li[1]

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Outline

- Splitting methods: numerically hard, large scale problems (particularly successful for relaxations of hard nonlinear discrete optimization problems.)
- We consider a Restricted Dual Peaceman-Rachford Splitting Method with strengthened bounds for a DNN relaxation; and we solve many *NP*-hard problems to (provable) optimality
- Here: quadratic assignment problem, QAP, a fundamental HARD combinatorial optimization problems; QAP models many real-life problems such as facility location, VLSI design.

Outline II

Exploiting Structure/Novel

- We use facial reduction, FR, to obtain a natural splitting of variables into cone/polyhedral constraints.
- We modify the subproblems by adding redundant constraints.
- We us provable lower and upper bounds.
- We modify dual variable update by exploiting scaling.
- We present extensive numerical experiments. In many instances the DNN relaxation resulted in the global optimal solution of the QAP.

Our Main Reference

A Restricted Dual Peaceman-Rachford Splitting Method for a Strengthened DNN Relaxation for QAP,

Graham/Hu/Im/Li/Wolkowicz in INFORMS J. Comput. 2022.

Further historical and current references are in the paper.

QAP, Quadratic Assignment Problem

Facility Location

Given: n facilities and n locations;
distance B_{st} between locations s, t;
flow $A_{i,j}$ between facilities i, j;
location (building) cost C_{is} facility i in location s.
$X = X_{ij} \in \Pi$ permutation matrix unkown $0, 1$ variables
$X(:) \in \mathbb{R}^{n^2}$, $n = 30$ instances still considered hard

trace formulation, $\langle Y, X \rangle = \mathrm{trace}(YX^T)$

minimize total flow and location costs

$$p^*_{\mathrm{QAP}} := \min_{X \in \Pi} \langle AXB - 2C, X \rangle,$$

Matrix Lifting to $\mathbb{S}^{n^2+1}$

$X \in \mathbb{R}^{n\times n}$; $x = \operatorname{vec}(X) \in \mathbb{R}^{n^2}$ (columnwise)

$$Y := \begin{pmatrix} 1 \\ x \end{pmatrix} \begin{pmatrix} 1 & x^T \end{pmatrix} \in \mathbb{S}^{n^2+1}$$

Block Representation

Indexing the rows and columns of Y from 0 to n^2,

$$Y = \begin{bmatrix} Y_{00} & \bar{y}^T \\ \bar{y} & \overline{Y} \end{bmatrix}, \quad \bar{y} = \begin{bmatrix} Y_{(10)} \\ Y_{(20)} \\ \vdots \\ Y_{(n0)} \end{bmatrix}, \quad \overline{Y} = xx^T = \begin{bmatrix} \overline{Y}_{(11)} & \overline{Y}_{(12)} & \cdots & \overline{Y}_{(1n)} \\ \overline{Y}_{(21)} & \overline{Y}_{(22)} & \cdots & \overline{Y}_{(2n)} \\ \vdots & \ddots & \ddots & \vdots \\ \overline{Y}_{(n1)} & \ddots & \ddots & \overline{Y}_{(nn)} \end{bmatrix}$$

where

$$\overline{Y}_{(ij)} = X_{:i} X_{:j}^T \in \mathbb{R}^{n\times n}, \forall i,j = 1,\ldots,n, \quad Y_{(j0)} \in \mathbb{R}^n, \forall j = 1,\ldots,n$$

Reformulation of QAP

Lifted Objective

$$L_Q := \begin{bmatrix} 0 & -(\mathrm{vec}\,(C)^T) \\ -\mathrm{vec}\,(C) & B \otimes A \end{bmatrix}, \qquad (\otimes \text{ is Kronecker product})$$

Lifted QAP

$$\begin{aligned} p^*_{\mathrm{QAP}} = \min \quad & \langle AXB - 2C, X \rangle = \langle L_Q, Y \rangle \\ \text{s.t.} \quad & Y := \begin{pmatrix} 1 \\ x \end{pmatrix} \begin{pmatrix} 1 \\ x \end{pmatrix}^T \in \mathbb{S}^{n^2+1}_+ \\ & X = \mathrm{Mat}\,(x) \in \Pi, \end{aligned}$$

where $\mathrm{Mat} = \mathrm{vec}^*$, the adjoint transformation.

Quadratic Constraints; Facial Reduction, FR

Characterizing Permutation Matrices

$$\|Xe - e\|^2 = \|X^T e - e\|^2 = 0,\ X \circ X = X,\ X^T X = XX^T = I,$$

$\circ$ is Hadamard product; e is vector of all ones.

Facial reduction FR using $Xe - e = IXe - e = 0$

Let $x = \mathrm{vec}(X)$; $y = \begin{pmatrix} 1 \\ x \end{pmatrix}$, $Y = yy^T$

We have $IXe = (e^T \otimes I)\mathrm{vec}(X)$ and

$$\begin{aligned} Xe - e = 0 \quad &\iff \quad y^T \begin{bmatrix} -e \\ (e^T \otimes I) \end{bmatrix} = 0 \\ &\iff \quad Y \left(\begin{bmatrix} -e \\ (e^T \otimes I) \end{bmatrix} \begin{bmatrix} -e \\ (e^T \otimes I) \end{bmatrix}^T \right) = 0 \end{aligned}$$

We have an exposing matrix and can do FR, $Y = \widehat{V} R \widehat{V}^T$.

FR Model; Simplified; Regularized

After FR, $Y = \widehat{V} R \widehat{V}^T$; Primal-Dual Strong Duality Holds

smaller, greatly simplified, many constraints are redundant:

$$
\text{(SDP)} \qquad \begin{array}{cl} \min\limits_{R} & \langle \widehat{V}^T L_Q \widehat{V}, R \rangle \\ \text{s.t.} & \mathcal{G}_{\bar{J}}(\widehat{V} R \widehat{V}^T) = u_0 \quad \text{(0-unit vector)} \\ & R \in \mathbb{S}_+^{(n-1)^2+1}. \end{array}
$$

$\mathcal{G}_{\bar{J}}(\cdot)$ so-called *gangster operator* ([6] ZKRW'94)

fixes the elements in set $\bar{J}$.

Details: $\widehat{V}$, Facial Reduction

$\widehat{Y}$

barycenter of set of feasible lifted Y of rank one for the SDP relaxation;

$\widehat{V} \in \mathbb{R}^{(n^2+1)\times((n-1)^2+1)}$

have orthonormal columns that span the range of $\widehat{Y}$ (explicit representation is available)

Minimal Face

every feasible Y of the SDP relaxation is contained in the minimal face, $\mathcal{F}$ of $\mathbb{S}_+^{n^2+1}$:

$$\mathcal{F} = \widehat{V}\mathbb{S}_+^{(n-1)^2+1}\widehat{V}^T \trianglelefteq \mathbb{S}_+^{n^2+1};$$

$$Y \in \mathcal{F}(\in \operatorname{ri}(\mathcal{F})) \implies \operatorname{Range}(Y) \subseteq (=) \operatorname{Range}(\widehat{V}),$$

Details: Gangster Operator $\mathcal{G}_{\bar{J}}$

linear map $\mathcal{G}_{\bar{J}} : \mathbb{S}^{n^2+1} \to \mathbb{R}^{|\bar{J}|}$; (shoots holes in the matrix)

By abuse of notation, also from $\mathbb{S}^{n^2+1}$ to $\mathbb{S}^{n^2+1}$, depending on the context:

$$\mathcal{G}_{\bar{J}} : \mathbb{S}^{n^2+1} \to \mathbb{S}^{n^2+1}, \quad \left[\mathcal{G}_{\bar{J}}(Y)\right]_{ij} = \begin{cases} Y_{ij} & \text{if } (i,j) \in \bar{J} \text{ or } (j,i) \in \bar{J}, \\ 0 & \text{otherwise.} \end{cases}$$

Gangster index set $\bar{J}$

union of the top left index (00) with set of indices $J, i < j$ in submatrix $\overline{Y} \in \mathbb{S}^{n^2}$:

(a) the off-diagonal elements in the n diagonal blocks in $\overline{Y}$

(b) the diagonal elements in the off-diagonal blocks in $\overline{Y}$

Many of these are redundant; still used in subproblems.

Doubly Nonnegative Relaxation, DNN

Motivated by natural splitting of variables from FR

Y - in polyhedral constraints subproblem
R - in SDP constraints subproblem

$$
(\text{DNN}) \qquad \begin{array}{lll} \min\limits_{R,Y} & \langle L_Q, Y\rangle & \\ \text{s.t.} & Y = \widehat{V} R \widehat{V}^T & (\text{splitting}) \\ & \mathcal{G}_{\bar{J}}(Y) = u_0 & (\text{polyhedral}) \\ & 0 \le Y \le 1 & (\text{polyhedral}) \\ & R \succeq 0 & (\text{convex cone}) \end{array}
$$

And, add redundant constraints to polyhedral and cone constraints.

Redundant Constraints Added to Subproblems

Let $Y \in \mathbb{S}^{n^2+1}$ be blocked as above.

Linearizations of Orthogonality: $XX^T = X^TX = I$

- $\mathrm{b^o diag}(Y) : \mathbb{S}^{n^2+1} \rightarrow \mathbb{S}^n$, sum of $n \times n$ diagonal blocks of Y:

$$\mathrm{b^o diag}(Y) := \sum_{k=1}^{n} Y_{(kk)} = I_n$$

- $\mathrm{o^o diag}(Y) : \mathbb{S}^{n^2+1} \rightarrow \mathbb{S}^n$: traces of blocks $\overline{Y}_{(ij)}$:

$$\mathrm{o^o diag}(Y) := \left(\mathrm{trace}\left(\overline{Y}_{(ij)}\right)\right) = I_n$$

More Redundant Constraints

Linearizations of $0, 1, X_{ij}^2 - X_{ij} = 0$

$\text{arrow}(Y) : \mathbb{S}^{n^2+1} \to \mathbb{R}^{n^2+1}$; difference of first column and diagonal of Y:

$$\text{arrow}(Y) := \left(Y_{(:1)} - \operatorname{diag}(Y)\right) = 0$$

trace constraint

By commutativity of the trace operator and $\widehat{V}^T \widehat{V} = I$:

$$\text{trace}(R) = \text{trace}(R\widehat{V}^T\widehat{V}) = \text{trace}\left(\widehat{V}R\widehat{V}^T\right) = \text{trace}(Y) = n + 1.$$

Set Constraints

Cone constraints

$$\mathcal{R} := \left\{ R \in \mathbb{S}^{(n-1)^2+1} : R \succeq 0,\ \operatorname{trace}(R) = n+1 \right\},$$

Polyhedral constraints

$$\begin{aligned} \mathcal{Y} : \quad = \quad & \Big\{ Y \in \mathbb{S}^{n^2+1} : \mathcal{G}_{\bar{J}}(Y) = u_0, 0 \le Y \le 1, \\ & \qquad \mathrm{b^\circ diag}(Y) = I,\ \mathrm{o^\circ diag}(Y) = I,\ \mathrm{arrow}(Y) = 0 \} \end{aligned}$$

Main Model

(Split) Model

$$(\mathrm{DNN}) \qquad \begin{array}{rcll} p^*_{\mathrm{DNN}} & := & \min\limits_{R,Y} & \langle L_Q, Y\rangle \\ & & \text{s.t.} & Y = \widehat{V} R \widehat{V}^T \\ & & & R \in \mathcal{R} \\ & & & Y \in \mathcal{Y}. \end{array}$$

Recovering original X from $\mathcal{Y}$ with redundant constraints

$Y \in \mathcal{Y} \implies X = \mathrm{Mat}\,(\mathit{diagonal}(Y)) = \mathrm{Mat}\,(\mathit{Row}1(Y))$ satisfy $Xe = X^T e = e$; (so doubly stochastic)

Optimality Conditions

Lagrangian function, dual variable Z

$$\mathcal{L}(R, Y, Z) = \langle L_Q, Y \rangle + \langle Z, Y - \widehat{V} R \widehat{V}^T \rangle.$$

Strictly feasibility/onto $\hat{R} \succ 0$, $\hat{Y} = \widehat{V} \hat{R} \widehat{V}$ holds

first order optimality conditions:

$$\begin{aligned} 0 &\in -\widehat{V}^T Z \widehat{V} + \mathcal{N}_{\mathcal{R}}(R), && \text{(dual } R \text{ feasibility)} && \text{(1a)} \\ 0 &\in L_Q + Z + \mathcal{N}_{\mathcal{Y}}(Y), && \text{(dual } Y \text{ feasibility)} && \text{(1b)} \\ Y &= \widehat{V} R \widehat{V}^T, \quad R \in \mathcal{R},\ Y \in \mathcal{Y}, && \text{(primal feasibility)} && \text{(1c)} \end{aligned}$$

where $\mathcal{N}_{\mathcal{R}}(R)$ (resp. $\mathcal{N}_{\mathcal{Y}}(Y)$) is normal cone to $\mathcal{R}$ (resp. $\mathcal{Y}$) at R (resp. Y).

Characterization of Optimality; Stopping Criteria

For subproblems

The primal-dual R, Y, Z are optimal if, and only if, normal cone conditions hold if, and only if,

$$R = \mathcal{P}_{\mathcal{R}}(R + \widehat{V}^T Z \widehat{V}) \tag{2a}$$

$$Y = \mathcal{P}_{\mathcal{Y}}(Y - L_Q - Z) \tag{2b}$$

$$Y = \widehat{V} R \widehat{V}^T. \tag{2c}$$

Dual Multiplier Z

Exploit structure

Let

$$\begin{array}{rcl} \mathcal{Z}_A & := & \left\{ Z \in \mathbb{S}^{n^2+1} : (Z + L_Q)_{ij} = 0, \forall i,j \text{ (in arrow positions)}, \right. \\ & & \left. \text{and } \forall ij \in J_R \text{ (redundant gangster positions)} \right\}. \end{array}$$

Modified PRSM Algorithm

(restricted contractive Peaceman-Rachford splitting; redundant constraints in subproblems; modified dual variable)

Augmented Lagrangian function

$$\mathcal{L}_A(R, Y, Z) = \langle L_Q, Y \rangle + \langle Z, Y - \widehat{V} R \widehat{V}^T \rangle + \frac{\beta}{2} \left\| Y - \widehat{V} R \widehat{V}^T \right\|_F^2,$$

where β is a positive penalty parameter.

Dual variable Z

$\mathcal{Z}_0 := \{Z \in \mathbb{S}^{n^2+1} : Z_{i,i} = 0,\ Z_{0,i} = Z_{i,0} = 0,\ i = 1, \ldots, n^2\}$
$\mathcal{P}_{\mathcal{Z}_0}$ projection onto $\mathcal{Z}_0$

PRSM for DNN

- **Initialize:** $\mathcal{L}_A$ is augmented Lagrangian; $\gamma \in (0, 1)$ is under-relaxation parameter; $\beta \in (0, \infty)$ is penalty parameter; $\mathcal{R}$,$\mathcal{Y}$ are subproblem sets; Y^0; and $Z^0 \in \mathcal{Z}_A$;

WHILE tolerances not met **DO**

- $R^{k+1} = \text{argmin}_{R \in \mathcal{R}} \mathcal{L}_A(R, Y^k, Z^k)$
- $Z^{k+\frac{1}{2}} = Z^k + \gamma\beta \cdot \mathcal{P}_{\mathcal{Z}_0}\left(Y^k - \widehat{V}R^{k+1}\widehat{V}^T\right)$
- $Y^{k+1} = \text{argmin}_{Y \in \mathcal{Y}} \mathcal{L}_A(R^{k+1}, Y, Z^{k+\frac{1}{2}})$
- $Z^{k+1} = Z^{k+\frac{1}{2}} + \gamma\beta \cdot \mathcal{P}_{\mathcal{Z}_0}\left(Y^{k+1} - \widehat{V}R^{k+1}\widehat{V}^T\right)$

ENDWHILE

Robustness/Convergence

Algorithm outline/remarks

- alternate minimization of variables R and Y interlaced by the dual variable Z update;
- R-update and the Y-update in are well-defined subproblems with unique solutions;
- many of the constraints are redundant in the SDP part but not within the subproblems; this improves rate of convergence and quality of Y when stopping early.
- modified dual update Z both after R-update and Y-update.

Theorem

Let $\{R^k\}, \{Y^k\}, \{Z^k\}$ be the sequences generated by the algorithm Then the sequence $\{(R^k, Y^k)\}$ converges to a primal optimal pair (R^*, Y^*), and $\{Z^k\}$ converges to an optimal dual solution $Z^* \in \mathcal{Z}_A$.

R-subproblem

$$\mathcal{R} := \left\{ R \in \mathbb{S}_+^{(n-1)^2+1} : \mathrm{trace}(R) = n+1 \right\}.$$

- $\mathcal{P}_{\mathcal{R}}(W)$ projection of W onto $\mathcal{R}$
- completing the square at current Y^k, Z^k: the R-subproblem can be explicitly solved by the projection operator $\mathcal{P}_{\mathcal{R}}$ as follows:

$$\begin{aligned} R^{k+1} &= \underset{R \in \mathcal{R}}{\mathrm{argmin}} \, -\langle Z^k, \widehat{V} R \widehat{V}^T \rangle + \frac{\beta}{2} \left\| Y^k - \widehat{V} R \widehat{V}^T \right\|_F^2 \\ &= \underset{R \in \mathcal{R}}{\mathrm{argmin}} \, \frac{\beta}{2} \left\| Y^k - \widehat{V} R \widehat{V}^T + \frac{1}{\beta} Z^k \right\|_F^2 \\ &= \underset{R \in \mathcal{R}}{\mathrm{argmin}} \, \frac{\beta}{2} \left\| R - \widehat{V}^T (Y^k + \frac{1}{\beta} Z^k) \widehat{V} \right\|_F^2 \\ &= \mathcal{P}_{\mathcal{R}}(\widehat{V}^T (Y^k + \frac{1}{\beta} Z^k) \widehat{V}) \end{aligned}$$

- Eigendecomposition and projection onto simplex.

Y-Subproblem

$\mathcal{Y} := \{Y \in \mathbb{S}^{n^2+1} : \mathcal{G}_{\bar{J}}(Y) = u_0,\ 0 \le Y \le 1,\ \mathrm{b^o diag}(Y) = I,\ \mathrm{o^o diag}(Y) = I,\ \mathrm{arrow}(Y) = 0\}$

• $\mathcal{P}_{\mathcal{Y}}(W)$ projection of W onto $\mathcal{Y}$

• completing the square at current $R^{k+1}, Z^{k+\frac{1}{2}}$: the Y-subproblem can be explicitly solved by the projection operator $\mathcal{P}_{\mathcal{Y}}$ as follows:

$$
\begin{aligned}
Y^{k+1} &= \operatorname*{argmin}_{Y \in \mathcal{Y}} \langle L_Q, Y\rangle + \langle Z^{k+\frac{1}{2}}, Y - \widehat{V} R^{k+1} \widehat{V}^T \rangle \\
&\qquad + \frac{\beta}{2} \left\| Y - \widehat{V} R^{k+1} \widehat{V}^T \right\|_F^2 \\
&= \operatorname*{argmin}_{Y \in \mathcal{Y}} \frac{\beta}{2} \left\| Y - \left(\widehat{V} R^{k+1} \widehat{V}^T - \frac{1}{\beta}(L_Q + Z^{k+\frac{1}{2}}) \right) \right\|_F^2 \\
&= \mathcal{P}_{\mathcal{Y}} \left(\widehat{V} R^{k+1} \widehat{V}^T - \frac{1}{\beta} \left(L_Q + Z^{k+\frac{1}{2}} \right) \right)
\end{aligned}
$$

• shooting holes; rounding to $0, 1$

Provable Lower Bounds from Approximate Solutions

$g(Z) := \min_{Y \in \mathcal{Y}} \langle L_Q + Z, Y \rangle - (n+1)\lambda_{\max}(\widehat{V}^T Z \widehat{V})$

where $\lambda_{\max}(\widehat{V}^T Z \widehat{V})$ denotes largest eigenvalue of $\widehat{V}^T Z \widehat{V}$.

Theorem

$d_Z^* := \max_Z g(Z)$ *is a concave maximization problem. Furthermore, strong duality holds with main* DNN *problem:*

$$p^*_{\mathbf{DNN}} = d_Z^*, \text{ and } d_Z^* \text{ is attained.}$$

Z dual feasible $\implies$ $g(Z)$ is a provable lower bound

Upper Bound from Nearest Permutation Matrix

Seemingly quadratic nearest discrete problem is a simplest LP

Given $\bar{X} \in \mathbb{R}^{n \times n}$

$$X^* = \operatorname*{argmin}_{X \in \Pi} \frac{1}{2}\|X - \bar{X}\|_F^2 = \operatorname*{argmin}_{X \in \Pi} -\langle \bar{X}, X \rangle = \operatorname*{argmin}_{X \in \mathcal{D}} -\langle \bar{X}, X \rangle,$$

since Von Neumann-Birkoff Theorem implies extreme points of doubly stochastic $\mathcal{D}$ are the permutation matrices Π; so can apply a simplex method or Hungarian method for assignment problem.

Upper bound

a feasible solution $X^* \in \Pi$ to the original QAP, gives a valid upper bound $\operatorname{trace}(AX^*B(X^*)^T)$.

Randomized Upper Bound

Previous Approaches using an approximate optimum Y^{out}

(Exploit Perron-Frobenius to conclude $v_1 \geq 0$.)

1. $\mathrm{vec}\,(\bar{X}) \cong$ col. 1(Y^{out}); find nearest $X^* \in \Pi$.
2. $Y^{\text{out}} = \sum_{i=1}^{r} \lambda_i v_i v_i^T$ spectral decomposition, $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_r > 0$; wlog $v_i \in \mathbb{R}^{n^2}$; $\mathrm{vec}\,(\bar{X}) = \lambda_1 v_1$; find nearest $X^* \in \Pi$.

Goemans-Williams type approximation algorithm, [3]

•$\xi \in (0,1)^r$; in decreasing order; perturb eigenvalues;
•$\mathrm{vec}\,(\bar{X}) = \sum_{i=1}^{r} \xi_i \lambda_i v_i.$; find nearest $X^* \in \Pi$.
• repeat $\max\{1, \min(3 * \lceil \log(n) \rceil, \text{ubest} - \text{lbest}\}$ number of times; 'ubest' and 'lbest' best current upper and lower bounds

Numerical Experiments with PRSM

improved performance with PRSM : cnvrgnce rates; rel. gap

• [4, ADMM] Oliveira/W./Xu, ADMM for the SDP relaxation of the QAP, Math. Program. Comput., 10 (2018).
• recent: relaxation methods [1, C-SDP], [2, F2-RLT2-DA] and [5, SDPNAL].

sizes n: small, medium, large

$$n \in \{10, \dots, 20\}, \{21, \dots, 40\}, \{41, \dots, 64\}.$$

$n = 64 : t(n^2 + 1) = 8,394,753$ variables;
nonnegativity cuts; SDP constraints

Conclusion

- We introduced a strengthened splitting method for solving the facially reduced DNN relaxation for the QAP.
- Our strengthened model and algorithm incorporates redundant constraints to the model that are not redundant in the subproblems; more specifically, the trace constraint in R-subproblem and projection onto doubly stochastic matrices in Y-subproblem.
- We exploit the structure of dual optimal multipliers and provide customized dual updates; leads to a new strategy for strengthening the provable lower bounds.
- codes can be downloaded with link `https://www.math.uwaterloo.ca/%7Ehwolkowi/henry/reports/ADMMnPRSMcodes.zip`.

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Thanks for your attention!

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