Hard Combinatorial Problems, Doubly Nonnegative Relaxations, Facial Reduction, and Alternating Direction Method of Multipliers

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Main References and Collaborators

- [7] F. Burkowski, J. Im, and H. Wolkowicz, *A Peaceman-Rachford splitting method for the protein side-chain positioning problem*, 2020.
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- [9] N. Graham, H. Hu, J. Im, X. Li, and H. Wolkowicz, *A restricted dual Peaceman-Rachford splitting method for QAP*, Tech. report, Waterloo, Ontario, 2020.
- [10] X. Li, T.K. Pong, H. Sun, and H. Wolkowicz, *A strictly contractive Peaceman-Rachford splitting method for the doubly nonnegative relaxation of the minimum cut problem*, Comput. Optim. Appl. **78** (2021), no. 3, 853–891. MR4221619

Outline/Background/Motivation I

- Solving hard combinatorial/discrete optimization problems requires: efficient upper/lower bounding techniques.
- These problems are often MODELLED using quadratic objectives and/or quadratic constraints, i.e., QQPs.
- Lagrangian relaxations of QQPs lead to Semidefinite Programming, SDP, and SDP relaxations, e.g., Handbooks on SDP [13, 1].
- SDP relaxations are expensive to solve using interior-point approaches. This becomes *doubly* expensive when cutting planes are added, e.g., using Doubly Nonnegative, DNN, relaxations

Outline/Background/Motivation II

- Strict feasibility fails for many of the SDP relaxations of these hard combinatorial problems.
  (Compare Rademacher Theorem: Loc. Lip. functions are differentiable a.e.)
  Facial reduction, FR , e.g., [3, 4, 5, 8] provides a means of regularizing the SDP relaxations.

- FR appears to provide a natural splitting of variables for the application of Alternating Direction Method of Multipliers, ADMM , type methods for large scale problems;
  and for exploiting structure.

- Classes of Problems:
  QAP ; Maxcut; Graph Partitioning;
  Min-Cut (application to SIDE-CHAIN POSITIONING)

Important Subproblem of Protein Structure Prediction:

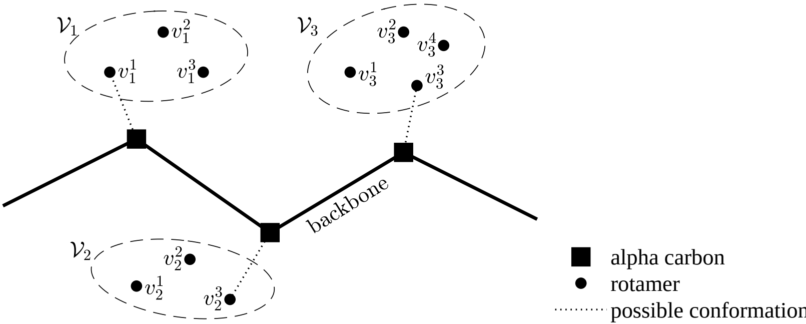

Figure: Diagram of Protein Side-Chain Positioning Problem, SCP

Biological Preamble

Side chain positioning (SCP)

- Given: constituent atoms of a protein;
  the side chain positioning (SCP) problem
  is one of the multiple subproblems of the hard problem of predicting a protein's three dimensional structure.
- Our protein macromolecule is a chain of amino acids, also called reisdues.

Amino acid is characterized by composition of its side chain

- amino acid consists of an "alpha" carbon atom ($-C_\alpha-$), and three components attached to it:
  -(i) amino group ((H_2N-);
  -(ii) carboxyl group ($-COOH$);
  -(iii) atom group called a side chain

Famous protein folding problem

Outline:

For tractability, accurate prediction of all atomic positions for folded minimal energy conformation typically uses:

1. calculate the positions of atoms in the backbone (e.g., homology modeling; fold recognition techniques)
2. given the positions of backbone atoms, calculate the conformations of all side chains, SCP.

Rotamericity/discretization of side chain conformations

- side chain typically adopts a conformation close to one of finitely many possible dihedral angles; each of the finite number of three dimensional conformations is called a rotamer.
- the more complicated side chains have rotamer sets with as many as 81 members for the twenty amino acids that make up proteins.

Modelling

$\mathcal{G} = (\mathcal{V}, \mathcal{E}, E)$ weighted, undirected graph

- node set $\mathcal{V} = \bigcup_{i=1}^{p} \mathcal{V}_i$, $\mathcal{V}_i$ subset of rotamers for i-th amino acid side chain/residue position,
  p is the number of residues.
- edge set $\mathcal{E}$; weights (energy between rotamers) E_{uv} for edge $uv \cong (u, v) \in \mathcal{E}$; E_{uu} is energy between backbone and chosen rotamer u.

Further: SDP notation

- $\mathcal{S}^t$, $t \times t$ real symmetric matrices, trace inner-product $\langle S, T \rangle = \operatorname{trace} ST$; Löwner partial order $S \succeq T$, $S \succ T$.
- for $v \in \mathbb{R}^s$, corresp. diagonal matrix is $\operatorname{Diag}(v) \in \mathcal{S}^s$
  adjoint linear transformation is $\operatorname{Diag}^*(S) = \operatorname{diag}(S) \in \mathbb{R}^s$
  the adjoint satisfies $\langle \operatorname{diag}(S), v \rangle = \langle S, \operatorname{Diag}(v) \rangle$
- $\bar{e} = \bar{e}_p$ ones vector; $\bar{E} = \bar{E}_k = \bar{e}_k \bar{e}_k^T$ ones matrix

Model details

global minimum-energy conformation (GMEC)

Choose one rotamer from each set $\mathcal{V}_i$; minimize sum of weights/energies on edges in E.

- $m := \begin{pmatrix} m_1 & \dots & m_p \end{pmatrix}^T$ size of subsets $\mathcal{V}_i$.
- $n_0 = |\mathcal{V}| \,(= \sum_k m_k)$
- $n := n_0 + 1$ size of matrices in SDP relaxation.

Quadratic integer programming (QIP) model

Computing the GMEC, a QIP

$$\begin{array}{rlll} val_{QIP} = & \min\limits_{x} & \sum\limits_{(u,v)\in\mathcal{E}} E_{uv} x_u x_v & \text{(quadr. form)} \\ & \text{s.t.} & \sum\limits_{u\in\mathcal{V}_k} x_u = 1, & \text{(linear)} \quad \forall\, k = 1, \ldots, p, \\ & & x_u \in \{0, 1\}, & \text{(hard constr)} \quad \forall u \in \mathcal{V}, \end{array}$$

$$x_u = \begin{cases} 1 & \text{if rotamer } u \text{ is chosen} \\ 0 & \text{otherwise} \end{cases}$$

Move onto Modelling and Duality

- We have seen an example/application (one of MANY) of where an IQP, Integer Quadratic Program, arises.
- These are NP-hard problems.
- move onto next step in solving such problems.

Hard Combinatorial Problems and Modelling with Quadratic Functions; Importance of Duality

Instance /Modelling with Quadratic Functions

$$\begin{array}{rll} \min & q_0(x) & (= x^T H x + 2g^T x + \alpha) \\ \text{s.t.} & Ax = b & \text{(linear constraint)} \\ & x \in K \subseteq \mathbb{R}^N & (K \text{ hard constraints}) \end{array}$$

Hard (Combinatorial) Constraints: e.g.,

- both $0, 1$ and ± 1 modelled with quadratic const., resp.,

$$\begin{array}{ccc} K := \{0,1\}^N & \text{or} & K := \{\pm 1\}^N \\ q_i(x) := x_i^2 - x_i = 0, \forall i & \text{or} & q_i(x) := x_i^2 - 1 = 0, \forall i \end{array}$$

- K is partition matrices, $x \in \mathcal{M}_m$, (GP)
- K is permutation matrices, $x \in \Pi_n$, (QAP)

Can Close the Duality Gap by Changing Model

Example: (Lagrangian) Duality Gap for QP

$$\begin{aligned} 1 = p^* &= \max\{-x_1^2 + x_2^2 : x_2 = 1\} \\ &< \infty = d^* \\ &= \inf_\lambda \max_x L(x,\lambda) = -x_1^2 + x_2^2 - \lambda(x_2 - 1) \end{aligned}$$

BUT with a Model Change (same problem!)

$$\begin{aligned} 1 = p^* &= \max\left\{-x_1^2 + x_2^2 : \boxed{(x_2-1)^2 = 0}\right\} \\ &= d^* = \inf_\lambda \max_x \{-x_1^2 + x_2^2 - \lambda(x_2-1)^2\} \end{aligned}$$

since stationarity and the Lagrangian function value satisfy:

$$0 = 2x_2 - 2\lambda(x_2 - 1) \implies x_2 = \frac{\lambda}{\lambda - 1} \to 1;$$

$$L(x,\lambda) = x_2^2 - \lambda(x_2-1)^2 = \frac{\lambda^2}{(\lambda-1)^2} - \lambda\frac{1}{(\lambda-1)^2} = \frac{\lambda}{\lambda-1} \to 1$$

Further Ex.: Close Duality Gap (Eig Relax QAP)

- Let $A = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix}$, $B = \begin{bmatrix} 3 & 0 \\ 0 & 4 \end{bmatrix}$, $\quad X^* = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$

$$10 = p^* = \begin{array}{ll} \min & \operatorname{trace} AXBX^T \\ \text{s.t.} & XX^T = I,\ X \in \mathbb{R}^{n \times n} \end{array}$$

- $L(X, S) = \operatorname{trace} AXBX^T + \operatorname{trace} S(XX^T - I),\ S \in \mathcal{S}^n$
  $\operatorname{trace} AXBX^T = x^T(B \otimes A)x,\ x = \operatorname{vec} X$

Lagrangian dual is an SDP: $\qquad d^* = \max\limits_{S \in \mathcal{S}^n} \min\limits_{X} L(X, S)$

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$$10 = p^* > 9 = d^* = \begin{array}{ll} \max & -\operatorname{trace} S \\ \text{s.t.} & B \otimes A + I \otimes S \succeq 0, \quad S \in \mathcal{S}^n \end{array}$$

where $B \otimes A = \begin{bmatrix} 3 & 0 & 0 & 0 \\ 0 & 6 & 0 & 0 \\ 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 8 \end{bmatrix} \implies S_{11} \geq -3, S_{22} \geq -6$

Change Model; Add Redundant Constraint; Increase Number of Lagrange Dual Multipliers

Duplicate orthogonality constraint $X^TX = I, XX^T = I$

Add: $X^TX = I$ closes duality gap by exploiting the new Lagrange multipliers in $T \in \mathcal{S}^n$

$$10 = p^* = 10 = d^* = \begin{array}{ll} \max & \operatorname{trace} -S - T \\ \text{s.t.} & B \otimes A + I \otimes S + T \otimes I \succeq 0, \end{array}$$

Theorem (Anstreicher, W. '95, [2])

Strong duality holds for

$$\begin{array}{ll} \min & \operatorname{trace} AXBX^T \\ s.t. & XX^T = I, X^TX = I, \; X \in \mathbb{R}^{n \times n} \end{array}$$

QP: Obtain Strong Duality in General? A Modelling Issue

$H \in \mathcal{S}^n$, A, $m \times n, m < n$, K compact

Theorem (Poljak, Rendl, W. '95, [11])

$$\begin{array}{rcll} p^* & = & \max_x & \{q_0(x) := x^T H x + 2g^T x + \alpha : Ax = b, x \in K\} \\ & = & \max_x & \{q_0(x) : \|Ax - b\|^2 = 0, x \in K\} \\ & = & d^* & = \boxed{\min_\lambda} \phi(\lambda) \end{array}$$

where the dual functional is:

$$\phi(\lambda) := \max_{x \in K} L(x, \lambda) := q_0(x) - \lambda \|Ax - b\|^2$$

Summary: To strengthen the Lagrangian dual

- linear constraints $Ax - b = 0$ to quadratic $\|Ax - b\|^2 = 0$
- Add redundant constraints

Move onto Solving the Lagrangian Relaxation/Lifting

- We have seen that adding redundant constraints and *squaring* linear constraints can close the duality gap, strengthen the Lagrangian relaxation.
- The Lagrangian relaxation of a QQP is an SDP; and the dual of this SDP is the *lifted/linearized* SDP relaxation.
- Move onto liftings/relaxations.

Model with Quadratics Details; Homogenize, and Lift to Matrix Space

Homogenize using $x_0 \in \mathbb{R}$ with $x_0^2 - 1 = 0$

$$\begin{cases} \min q_0(x, x_0) = x^T H x + 2g^T x x_0 + \alpha x_0^2 \\ Ax - b = 0 \quad \cong \quad \|Ax - bx_0\|_2^2 = 0 \end{cases}$$

Lifting (linearization): $\mathbb{R}^{N+1} \rightarrow \mathbb{S}^{N+1}$

$$y = \begin{pmatrix} x_0 \\ x \end{pmatrix}, \; Y = yy^T \in \mathbb{S}_+^{N+1}, \quad \text{symmetric, psd,} \quad Y_{00} = 1$$

$$\text{obj. fn.} \quad y^T \begin{bmatrix} \alpha & g^T \\ g & H \end{bmatrix} y = \operatorname{trace} \begin{bmatrix} \alpha & g^T \\ g & H \end{bmatrix} Y, \qquad \operatorname{rank}(Y) = 1$$

Relaxation to Convex Problem:

Discard the (hard) rank one constraint on Y

Lifting with QQP and FACIAL REDUCTION

Lifting Linear Equality Constraint

$$\begin{aligned} 0 &= \|Ax - bx_0\|_2^2 = \left\| \begin{bmatrix} -b & A \end{bmatrix} \begin{pmatrix} x_0 \\ x \end{pmatrix} \right\|_2^2 \\ &= \begin{pmatrix} x_0 \\ x \end{pmatrix}^T \begin{bmatrix} -b^T \\ A^T \end{bmatrix} \begin{bmatrix} -b & A \end{bmatrix} \begin{pmatrix} x_0 \\ x \end{pmatrix} \\ &= \operatorname{trace} \begin{bmatrix} \|b\|^2 & -b^T A \\ -A^T b & A^T A \end{bmatrix} Y = 0 \end{aligned}$$

EXPOSING VECTOR $W \in \mathbb{S}_+^{N+1}$, with: spectr. decomp., FR

$$W := \begin{bmatrix} \|b\|^2 & -b^T A \\ -A^T b & A^T A \end{bmatrix} = \begin{bmatrix} V & U \end{bmatrix} \begin{bmatrix} 0 & 0 \\ 0 & D \end{bmatrix} \begin{bmatrix} V & U \end{bmatrix}^T, \; D \in \mathbb{S}_+^{N+1-r}$$

Y feasible $\implies$ $YW = 0$ (Strict feasibility (Slater) fails)

$\implies$ $Y = VRV^T, \; R \in \mathbb{S}_+^r$ (facial reduction)

Ex: Relaxation of 0, 1 Hard Discrete Constraint

Zero-One; Homogenize with x_0, $x_0^2 - 1 = 0$ ($Y_{00} = 1$)

$$q_i(x, x_0) := x_i^2 - x_i x_0 = 0, \ \forall i$$

Lifting (linearization): $\mathbb{R}^{N+1} \rightarrow \mathbb{S}^{N+1}$

$$y = \begin{pmatrix} x_0 \\ x \end{pmatrix}, \ Y = yy^T \in \mathbb{S}_+^{N+1}, \quad \text{symmetric, psd,} \quad Y_{00} = 1$$

$$\text{constr. for } \{0, 1\}: \quad \text{arrow}(Y) = e_0 := \begin{pmatrix} 1 \\ 0 \end{pmatrix} \in \mathbb{R}^{N+1}$$

$$(\text{diag}\,(Y) = Y_{:,0})$$

Adjoint: Arrow $\cong$ arrow*

$$\langle \text{Arrow}(v), S \rangle = \langle v, \text{arrow}(S) \rangle, \quad \forall v \in \mathbb{R}^{N+1}, \forall S \in \mathbb{S}^{N+1}$$

Move onto a Natural Splitting, FR

- We have modelled hard problems with quadratics, QQPs; we add redundant constraints when possible; after homogenization, we apply Lagrangian relaxation to get the SDP relaxation; we apply facial reduction, FR, and remove redundant constraints.
- The method of choice for SDP was/is primal-dual interior-point methods. However, they do not scale well, and have difficulty getting high accuracy. Adding cutting planes from e.g., nonnegativity constraints, DNN relaxations, makes the problems doubly hard numerically.
- Facial reduction, FR, appears to provide a natural splitting to be able to apply ADMM type first order methods.

Splitting Methods, Facial Reduction, FR, for DNN

Natural Splitting? $Y \in \mathcal{P},\ R \in \mathcal{R} \subseteq \mathbb{S}^r_+ \quad Y = VRV^T$

$$Y \in \mathcal{P} \subset \mathbb{S}^{N+1}_+, \qquad R \in \mathcal{R} \subseteq \mathbb{S}^r_+, \quad r < N+1$$

Facial reduction generally provides a reduction in dimension and a guarantee that strict feasibility holds.
There is a natural separation of constraints where

$$Y \in \mathcal{P} \text{ polyhedral} \qquad R \in \mathcal{R} \text{ convex set}$$

Adding Redundant Constraints Back

- FR results in many constraints becoming redundant; and these are deleted for e.g., interior-point methods.
- However, after the splitting, many of the redundant constraints can be added back to the separate split problems to form smaller sets $\mathcal{P}, \mathcal{R}$.

Instance: Minimum Cut, MC, Problem

Given: Undirected Graph $G = (\mathcal{V}, \mathcal{E})$, Adjacency Matrix A

edge set $\mathcal{E}$ and node set $|\mathcal{V}| = n$
$m = (m_1 \; m_2 \; \dots \; m_k)^T$, $\sum_{i=1}^{k} m_i = n$; given partition into k sets

MC Problem:

partition vertex set $\mathcal{V}$ into k subsets with given sizes in m
to *minimize the cut* after removing the k-th set;
X is the unknown $0, 1$ partition matrix.

Applications

re-orderings for sparsity patterns; microchip design and circuit board, floor planning and other layout problems.
($k = 3$, vertex separator problem)

Quadratic-Quadratic Model/Homogenized

Include Many Redundant Constraints; X a Partition Matrix

$$
\begin{array}{rclll}
\operatorname{cut}(m) & = & \min & \frac{1}{2}\operatorname{trace} AXBX^T & \text{quadr. form} \\
 & & \text{s.t.} & X \circ X = x_0 X & \in \{0,1\} \\
 & & & \|Xe - x_0 e\|^2 = 0 & \text{row sums } = 1 \\
 & & & \|X^T e - x_0 m\|^2 = 0 & \text{column sums} \\
 & & & X_{:i} \circ X_{:j} = 0, \ \forall i \neq j & \text{col. elem. orth.} \\
 & & & X^T X - M = 0 & \text{scaled orth.} \\
 & & & \operatorname{diag}(XX^T) - e = 0 & \text{unit norm rows} \\
 & & & x_0 e_n^T X e_k - n = 0 & n \text{ vertices} \\
 & & & x_0^2 = 1 & \text{homog.}
\end{array}
$$

- A adjacency; B structured for k-th set
- X, $n \times k$ partition matrix; cols are indicator vectors for sets
- e_j is the vector of ones of dimension j; $M = \operatorname{Diag}(m)$.
- $u \circ v$ Hadamard (elementwise) product.

SDP Constraints, FR and Exposing Vectors

Trace constraints (from linear equality constraints

$$\operatorname{trace} D_1 Y = 0, \qquad D_1 := \begin{bmatrix} n & -e_k^T \otimes e_n^T \\ -e_k \otimes e_n & (e_k e_k^T) \otimes I_n \end{bmatrix},$$

$$\operatorname{trace} D_2 Y = 0, \qquad D_2 := \begin{bmatrix} m^T m & -m^T \otimes e_n^T \\ -m \otimes e_n & I_k \otimes (e_n e_n^T) \end{bmatrix},$$

e_j vector of ones of dimension j; $D_i \succeq 0, i = 1, 2$; nullspaces of these matrices yield the facial reduction $Y = VRV^T$.

Block: trace, diagonal and off-diagonal

$$\begin{array}{rcl} \mathcal{D}_t(Y) & := & \left(\operatorname{trace} \overline{Y}_{(ij)}\right) = M \in \mathbb{S}^k; \\ \mathcal{D}_d(Y) & := & \sum_{i=1}^k \operatorname{diag} \overline{Y}_{(ii)} = e_n \in \mathbb{R}^n; \\ \mathcal{D}_o(Y) & := & \left(\sum_{s \neq t} \left(\overline{Y}_{(ij)}\right)_{st}\right) = \hat{M} \in \mathbb{S}^k, \end{array}$$

where $\hat{M} := mm^T - M$.

SDP Constraints cont. . .

Gangster constraints on Y are Strong

The Hadamard product and orthogonal type constraints lead to

gangster constraints

i.e., simple constraints that restrict elements to be zero (shoot holes in the matrix) and/or restrict entire blocks.
$(X_{:i} \circ X_{:j} = 0 \implies Y_{si,tj} = 0, \forall s, t)$
gangster and restricted gangster constraint on Y:

$$\mathcal{G}_H(Y) = 0,$$

for specific index sets H.

SDP Relaxation

SDP Relaxation with Many (some redundant) Constraints

$$
\begin{array}{rll}
\text{cut}(m) \geq p^*_{\text{SDP}} := & \min & \frac{1}{2} \operatorname{trace} L_A Y \\
& \text{s.t.} & \operatorname{arrow}(Y) = e_0 \\
& & \operatorname{trace} D_1 Y = 0, \ \operatorname{trace} D_2 Y = 0 \\
& & \mathcal{G}_{J_0}(Y) = 0, \ Y_{00} = 1 \\
& & \mathcal{D}_t(Y) = M, \ \mathcal{D}_d(Y) = e, \ \mathcal{D}_o(Y) = \widehat{M} \\
& & Y \in \mathbb{S}^{kn+1}_+
\end{array}
$$

Equivalent FR greatly simplified SDP; with $Y = \widetilde{V} R \widetilde{V}^T$

$$
\begin{array}{rcll}
\text{cut}(m) \geq p^*_{\text{SDP}} & = & \min & \frac{1}{2} \operatorname{trace} \left(\widetilde{V}^T L_A \widetilde{V} \right) R \\
& & \text{s.t.} & \mathcal{G}_{\hat{J}_{\mathcal{I}}}(\widetilde{V} R \widetilde{V}^T) = \mathcal{G}_{\hat{J}_{\mathcal{I}}}(e_0 e_0^T) \\
& & & R \in \mathbb{S}^{(k-1)(n-1)+1}_+
\end{array}
$$

Primal-Dual Strong Duality (Regularity) for FR SDP

Theorem

1. *(Generalized) slater point for the primal:*

$$\widetilde{R} = \left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & \frac{1}{n^2(n-1)}\left(n\mathrm{Diag}\left(\hat{m}_{k-1}\right) - \hat{m}_{k-1}\hat{m}_{k-1}^T\right) \otimes \left(nI_{n-1} - E_{n-1}\right) \end{array}\right] \in \mathbb{S}_{++}^{(k-1)(n-1)+1}.$$

   Moreover, Robinson regularity holds.

2. *The dual problem*

$$\begin{array}{ll} \max & \frac{1}{2} w_{00} \\ \text{s.t.} & \widetilde{V}^T \mathcal{G}^*_{\hat{J}_{\mathcal{I}}}(w) \widetilde{V} \preceq \widetilde{V}^T L_A \widetilde{V}. \end{array}$$

   satisfies strict feasibility.

Motivation for Splittings

Difficulties for Primal-dual interior-point Methods for SDP

- solving large problems
- obtaining high accuracy solutions
- exploiting sparsity
- adding on nonnegativity and other cutting plane constraints

First order operator splitting methods for SDP

- FR provides a natural (successful) splitting, $Y = VRV^T$, (Y polyhedral, R cone/convex)
- Flexibility in dealing with additional constraints
- separable/split optimization steps are inexpensive

Strengthen model with redundant constraint

Set Constraints, Low Rank (helps with early stopping)

$$\begin{aligned}\mathcal{R} &:= \{R \in \mathbb{S}_+^{(k-1)(n-1)+1} : \operatorname{trace} R = n+1\},\\ \mathcal{Y} &:= \{Y \in \mathbb{S}^{nk+1} : 1 \geq Y(J^c) \geq 0,\\ &\qquad \mathcal{G}_{\bar{J}}(Y) = \mathcal{G}_{\bar{J}}(e_0 e_0^T)\\ &\qquad \mathcal{D}_o(Y) = \widehat{M},\ e^T Y_{(i0)} = m_i, \forall i\}\end{aligned}$$

Strengthened model for Splitting Approach

$$(\text{DNN})\quad p^*_{DNN} = \begin{array}{ll}\min & \frac{1}{2}\operatorname{trace} L_A Y + \mathbb{1}_{\mathcal{Y}}(Y) + \mathbb{1}_{\mathcal{R}}(R)\\ \text{s.t.} & Y = \widehat{V} R \widehat{V}^T,\end{array}$$

where $\mathbb{1}_{\mathcal{S}}(\cdot)$ is indicator function of set $\mathcal{S}$.

Solve the DNN using the Splitting Method

Augmented Lagrangian Function, $\mathcal{L}_\beta(R, Y, Z) =$

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

- $\beta > 0$ penalty parameter for quadratic penalty term,
- (L_s diagonally scaled objective $L_s := \frac{1}{2}L + \alpha I \succ 0$)

$$f_{\mathcal{R}}(R) = \mathbb{1}_{\mathcal{R}}(R), \quad g_{\mathcal{Y}}(Y) = \operatorname{trace} L_s Y + \mathbb{1}_{\mathcal{Y}}(Y).$$

sPRSM, Strictly Contractive Peaceman-Rachford Splitting

i.e., alternate minimization of $\mathcal{L}_\beta$ in the variables Y and R interlaced by an update of the Z variable.
In particular, we update the dual variable Z both after the R-update *and* the Y-update (both of which have unique solutions).

FRSMR, FR Splitting Method with Redundancies

- Pick any $Y^0, Z^0 \in \mathbb{S}^{nk+1}$. Fix $\beta > 0$ and $\gamma \in (0,1)$.
- For each $t = 0, 1, \ldots,$ update

$$\begin{aligned}
\bullet R^{t+1} &= \operatorname{argmin}_{R \in \mathcal{R}} \mathcal{L}_\beta(R, Y^t, Z^t) \\
&= \operatorname{argmin}_R f_{\mathcal{R}}(R) - \langle Z^t, \widehat{V} R \widehat{V}^T \rangle + \frac{\beta}{2} \left\| Y^t - \widehat{V} R \widehat{V}^T \right\|^2 \\
\bullet Z^{t+\frac{1}{2}} &= Z^t + \gamma\beta(Y^t - \widehat{V} R^{t+1} \widehat{V}^T), \\
\bullet Y^{t+1} &= \operatorname{argmin}_{Y \in \mathcal{Y}} \mathcal{L}_\beta(R^{t+1}, Y, Z^{t+\frac{1}{2}}) \\
&= \operatorname{argmin}_Y g_{\mathcal{Y}}(Y) + \langle Z^{t+\frac{1}{2}}, Y \rangle + \frac{\beta}{2} \left\| Y - \widehat{V} R^{t+1} \widehat{V}^T \right\|^2, \\
\bullet Z^{t+1} &= Z^{t+\frac{1}{2}} + \gamma\beta(Y^{t+1} - \widehat{V} R^{t+1} \widehat{V}^T).
\end{aligned}$$

The argmins can be found explicitly.

Global convergence

Theorem

Let $\{R^t\}$, $\{Y^t\}$ and $\{Z^t\}$ be the generated sequences from FRSMR. *Then $\{(R^t, Y^t)\}$ converges to an optimal solution (R^*, Y^*) of the* DNN *relaxation, $\{Z^t\}$ converges to some Z^*, and (R^*, Y^*, Z^*) satisfies the optimality conditions of the* DNN *relaxation*

$$\begin{aligned} 0 &\in -\widehat{V}^T Z^* \widehat{V} + \mathcal{N}_{\mathcal{R}}(R^*), \\ 0 &\in L_s + Z^* + \mathcal{N}_{\mathcal{Y}}(Y^*), \\ Y^* &= \widehat{V} R^* \widehat{V}^T, \end{aligned}$$

where $\mathcal{N}_S(x)$ denotes the normal cone of S at x. □

1. Explicit solution for R^{t+1}

With the assumption that $\widehat{V}^T\widehat{V} = I$

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

where $\mathcal{P}_{\mathcal{R}}$ denotes the projection (nearest point) onto the intersection of the SDP cone $\mathbb{S}_+^{(k-1)(n-1)+1}$ and the hyperplane $\{R \in \mathbb{S}^{(k-1)(n-1)+1} : \operatorname{trace} R = n+1\}$.

(diagonalize; then project eigenvalues onto simplex)

2. Explicit solution of Y^{t+1}

The Y-subproblem yields a closed form solution by projection onto the polyhedral set $\mathcal{Y}$, i.e.,

$$Y^{t+1} = \operatorname{argmin}_{Y \in \mathcal{Y}} \frac{\beta}{2} \left\| Y - \boxed{\widehat{V} R^{t+1} \widehat{V}^T - \frac{1}{\beta}(L_s + Z^{t+\frac{1}{2}})} \right\|^2.$$

Note that the update (projection of $\tilde{Y}$) satisfies e.g.,

$$(Y^{t+1})_{ij} = \begin{cases} 1 & \text{if } i = j = 0 \\ 0 & \text{if } ij \in J \backslash \{00\} \\ 0 & \text{if } ij \in J^c,\ Y_{ij} \leq 0 \\ \tilde{Y}_{ij} & \text{if } ij \in J^c,\ 0 < Y_{ij}. \end{cases}$$

Lower bound from Inaccurate Solutions

Theorem (Fenchel Dual)

Define modified dual functional
$g(Z) := \min_{Y\in\widetilde{\mathcal{Y}}} \langle L_s + Z, Y\rangle - (n+1)\lambda_{\max}(\widehat{V}^T Z \widehat{V})$,
with $\widetilde{\mathcal{Y}} :=$

$$\{Y \in \mathbb{S}^{nk+1} : \mathcal{G}_{\hat{\mathcal{J}}_0}(Y) = \mathcal{G}_{\hat{\mathcal{J}}_0}(e_0 e_0^T),\ 0 \le \mathcal{G}_{\hat{\mathcal{J}}_0^c}(Y) \le 1,$$
$$\mathcal{D}_o(Y) = \widehat{M},\ \mathcal{D}_t(Y) = M,\ e^T Y_{(i0)} = m_i, i = 1, \dots, k\}.$$

Then

$$p^*_{\mathrm{DNN}} = d^*_Z := \max_Z g(Z),$$

and the latter (dual) problem is attained, i.e., strong duality holds. □

The Lower Bound

Evaluating $g(Z^t)$ always yields a lower bound for the DNN relaxation optimal value

$$p^*_{\mathrm{DNN}} \ge g(Z^t)$$

Upper bound from feasible solution

Approx. output Y^{out}

- Obtain a vector $v = (v_0 \ \bar{v})^T \in \mathbb{R}^{nk+1}$, $v_0 \neq 0$ from Y^{out}
- Reshape $\bar{v}$; get $n \times k$ matrix X^{out}
- Since X implies $\operatorname{trace} X^T X = n$, a constant, we get

$$\left\| X^{\text{out}} - X \right\|^2 = -2 \operatorname{trace} X^T X^{\text{out}} + \text{constant}.$$

- Solve the linear program (transportation problem)

$$\hat{X} \in \operatorname{argmax} \left\{ \langle X^{\text{out}}, X \rangle : Xe = e, X^T e = m, X \geq 0 \right\}$$

- Upper bound $= \frac{1}{2} \operatorname{trace} A\hat{X}B\hat{X}^T$

Choosing the vector v for X^{out} for upper bound

rank $Y = 1 \implies$ column/eigenvector 0 yields opt. X

1. column 0 of Y^{out};
2. eigenvector corresponding to largest eigenvalue of Y^{out};
3. random sampling/repeated: sum of random weighted-eigenvalue eigenvectors of Y^{out},
$$v = \sum_{i=1}^{r} w_i \lambda_i v_i,$$
where ordered eigenpairs of Y^{out} and ordered weights; r here is the *numerical rank* of Y^{out}.

Numerics; Protein Data Bank (PDB)

- MATLAB 2018b; Dell PowerEdge M630; two Intel Xeon E5-2637v3 4-core 3.5 GHz (Haswell); 64 Gigabyte. (times are reasonable)
- relative gaps are approx. 0; we have essentially solved the original NP-hard problem.

Table Headings:

- **problem**: instance name;
- **p**: number of amino acids;
- $\mathbf{n_0}$: total number of rotamers;
- **lbd**: lower bound;
- **ubd**: upper bound;
- **rel.gap**: relative gap;
- **iter**: number of iterations with tolerance $\epsilon = 10^{-10}$;
- **time(sec)**: CPU time (in seconds)

Numerics: Small PDB Instances; χ angles percent correct; rel-gap shows essentially global opt.

Problem Data				Numerical Results			Timing		χ angle	
#	name	p	n_0	lbd	ubd	rel-gap	iter	time(sec)	χ_1 angle	χ_{12} angle
1	1AIE	26	34	-46.95892	-46.95892	7.03672e-15	200	0.09	0.654	0.480
2	2ERL	34	103	55.33284	55.33284	5.61228e-14	300	5.52	0.588	0.476
3	1CBN	37	112	-40.42751	-40.42751	2.51561e-13	1652	33.40	0.821	0.727
5	1BX7	41	99	16.96026	16.96026	3.47516e-11	200	3.31	0.610	0.522
6	2FDN	42	51	-59.43092	-59.43092	2.45420e-14	100	0.01	0.738	0.583
7	1MOF	46	94	-79.05580	-79.05580	8.57412e-15	200	2.56	0.717	0.514
8	1CTF	47	74	-97.18893	-97.18893	1.28887e-13	100	0.82	0.766	0.639
9	1NKD	50	199	-51.78466	-51.78466	7.80603e-13	4845	282.37	0.700	0.659
10	2IGD	50	126	-78.50608	-78.50608	8.99352e-15	495	9.91	0.760	0.677
11	2SN3	53	112	-5.56818	-5.56818	4.78619e-12	600	10.95	0.736	0.541
12	1MSI	54	112	-87.46958	-87.46958	1.53466e-14	600	10.97	0.796	0.722
13	1AHO	54	140	24.66925	24.66925	7.76341e-15	1400	39.72	0.722	0.556
15	1CTJ	61	258	-103.32705	-103.32705	1.84748e-12	1919	143.33	0.902	0.679
16	1RZL	65	121	17.26470	17.26470	1.17993e-12	2177	42.27	0.831	0.758
17	1TIF	66	614	-155.17859	-155.17859	5.42223e-14	700	207.67	0.758	0.567
18	1BDO	69	221	-136.29933	-136.29933	3.94748e-15	500	27.28	0.855	0.646
19	1OPD	70	112	-139.64632	-139.64632	4.76581e-14	200	2.86	0.657	0.438
20	1VQB	75	406	-96.94940	-96.94940	2.24575e-14	700	93.15	0.824	0.611
21	1IUZ	75	221	-150.88238	-150.88238	4.31820e-15	3400	194.65	0.880	0.712
22	1ABA	76	376	-137.59962	-137.59963	1.35194e-11	400	46.04	0.895	0.734
23	1FNA	76	131	-172.01313	-172.01313	1.72989e-14	700	13.49	0.800	0.651
24	1CYO	78	220	-75.36668	-75.36668	1.33555e-13	500	27.53	0.833	0.639
26	2MCM	80	123	-135.14024	-135.14024	2.16748e-11	200	3.04	0.850	0.800
28	1A68	81	424	-178.12555	-178.12555	9.54680e-16	1000	142.07	0.840	0.662
30	2ACY	84	580	-146.32254	-146.32254	2.88432e-14	8200	2063.31	0.857	0.667
31	1BM8	85	687	-119.54537	-119.54537	3.55137e-16	1200	405.69	0.835	0.618
32	1BKF	89	339	-170.80514	-170.80514	1.24600e-13	1832	177.58	0.843	0.545
33	3CYR	91	137	-144.06405	-144.06405	1.42138e-11	1900	33.93	0.846	0.593
34	3VUB	92	544	-229.38312	-229.38312	4.94542e-15	900	205.25	0.804	0.574
35	1JER	96	462	-120.78401	-120.78400	6.02020e-13	3050	505.43	0.777	0.541
36	2HBG	97	275	-178.42210	-178.42210	4.28894e-15	300	21.82	0.825	0.520
37	1POA	97	470	278.08280	278.08280	8.16180e-14	4992	860.25	0.773	0.529
38	1C52	99	256	-223.31096	-223.31096	1.18101e-14	2700	172.67	0.828	0.690
39	2A0B	99	642	-161.45228	-161.45228	1.98309e-14	5400	1616.92	0.765	0.650

Numerics: Big PDB Instances; χ angles percent correct; rel-gap shows essentially global opt.

Problem Data				Numerical Results			Timing		χ angle	
#	name	p	n_0	lbd	ubd	rel-gap	iter	time(sec)	χ_1 angle	χ_{12} angle
96	1AL3	201	1077	119.66598	119.66598	5.10139e-12	12877	9773	0.791	0.549
97	1ARB	202	1466	-61.52823	-61.52823	1.22112e-13	7200	11157	0.851	0.693
99	1NLS	203	1060	-297.73578	-297.73578	3.50702e-14	2600	1851	0.818	0.603
100	1MRJ	208	1178	-295.13711	-295.13711	1.23056e-13	1931	1700	0.813	0.636
101	1OAA	208	854	-317.83422	-317.83422	2.39277e-14	2300	1012	0.803	0.680
102	2DRI	210	906	-398.45564	-398.45564	3.10608e-14	6400	3003	0.805	0.616
103	2CBA	223	1018	-86.52145	-86.52145	1.30549e-11	3200	1979	0.857	0.665
104	2POR	224	1304	-83.22221	-83.22221	8.82520e-12	12846	14255	0.830	0.642
105	3SEB	224	1412	77.15853	77.15852	3.38717e-13	267900	346506	0.782	0.592
106	1MLA	227	1322	-484.10542	-484.10542	1.87677e-14	40100	42801	0.815	0.617
107	1DCS	232	1170	-342.68600	-342.68600	1.65634e-14	4300	3519	0.817	0.609
108	1AKO	234	1387	-244.65691	-244.65691	1.39815e-13	5100	6209	0.808	0.605
109	1PDA	239	891	-423.50226	-423.50226	1.97074e-14	5500	2427	0.860	0.696
110	1EZM	239	1497	-217.36581	-217.36581	5.10340e-13	2000	3136	0.862	0.575
111	1C3D	243	1679	-400.69876	-400.69876	1.38850e-14	23900	85403	0.827	0.655
113	8ABP	245	1743	-273.90716	-273.90716	1.59505e-14	7100	27815	0.802	0.640
114	1CVL	246	910	-537.04249	-537.04249	4.37792e-14	7900	3525	0.850	0.711
115	1RYC	248	1831	-202.60568	-202.60568	1.11948e-15	12500	56371	0.802	0.561
116	1MRP	248	1648	-350.97062	-350.97062	5.27240e-14	11600	44124	0.754	0.596
117	1IXH	252	1134	-289.75241	-289.75241	1.37089e-14	1000	770	0.821	0.663
118	1FNC	253	1940	-310.60998	-310.60999	9.51745e-13	27600	151870	0.802	0.627
120	1SBP	256	1704	-271.08838	-271.08838	4.18600e-15	43300	170625	0.816	0.596
121	2CTC	264	1536	-213.88596	-213.88596	1.59617e-13	10000	34876	0.826	0.635
122	1PGS	265	2190	-16.14049	-16.14049	4.69696e-14	22800	156081	0.837	0.541
123	1MSK	271	1798	-162.50978	-162.50978	1.03393e-13	152200	606216	0.775	0.585
124	1BG6	271	784	-452.62383	-452.62383	3.17007e-13	13300	4072	0.819	0.640
125	1ARU	271	939	-314.40589	-314.40589	9.99588e-12	73500	33326	0.775	0.629
126	1A8E	274	1096	-249.85499	-249.85499	3.17872e-15	103700	68466	0.825	0.613
127	1AXN	278	2343	-300.34290	-300.34291	2.41852e-14	13400	105053	0.831	0.631
128	1TAG	279	1330	-253.22167	-253.22167	2.78928e-13	4200	4301	0.817	0.634
129	1ADS	280	1560	733.91440	733.91440	6.19197e-16	13000	46057	0.771	0.498
130	3PTE	284	2006	161.17216	161.17216	3.88515e-14	11000	58278	0.856	0.651
131	1CEM	292	2400	-24.20196	-24.20196	2.92824e-13	7100	55850	0.860	0.662

Conclusion

- We discussed strategies for finding new, strengthened lower and upper bounds, for hard discrete optimization problems.
- In particular, we exploited the fact that strict feasibility fails for many of these problems and that facial reduction, FR, leads to a natural splitting approach for ADMM, sPRSM, type methods.
- The FR makes many constraints redundant and simplifies the problem. We strengthened the subproblems in the splitting by *returning* redundant constraints.
- A special scaling, and a random sampling provided strengthened lower and upper bounds from low approximate solutions from our approach. (Allowing for early stopping.

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Further Numerical Tests from [10, 9, 7, 6]

Tests using:

Matlab R2017a on a ThinkPad X1 with an Intel CPU (2.5GHz) and 8GB RAM running Windows 10.

Three classes of problems:

(a) random structured graphs (compare with previous results in Pong et al. [12])

(b) partially random graphs with various sizes classified by the number of 1's, $|\mathcal{I}|$, in the vector m (similar to QAP)

(c) vertex separator instances

Facial Reduction, FR

Lifting Linear Equality Constraint

Table: Data terminology

imax	maximum size of each set
k	number of sets
n	number of nodes (sum of sizes of sets)
p	density of graph
u_0	known lower bound
$l = e^T m_{\text{one}}$	number of 1's in m
Iters	number of iterations
CPU	time in seconds
Bounds	best lower and upper bounds and relative gap
Residuals	*final* values of: $\left\Vert Y^{t+1} - \widehat{V} R^{t+1} \widehat{V}^T \right\Vert$ $(\cong \Delta Z)$; $\left\Vert Y^{t+1} - Y^t \right\Vert$ $(\cong \Delta Y)$

Comparison small structured graphs with Pong et al

Data				Lower bounds		Upper bounds		Rel-gap		Time (cpu)	
n	k	$\lvert E\rvert$	u_0	FRSMR	Mosek	FRSMR	Mosek	FRSMR	Mosek	FRSMR	Mosek
20	4	136	6	6	6	6	6	0.00	0.00	0.21	3.96
25	4	222	8	8	8	8	8	0.00	0.00	0.20	10.94
25	5	170	14	14	14	14	14	0.00	0.00	0.31	34.19
31	5	265	22	22	22	22	22	0.00	0.00	1.28	149.49

Numerics cont... Random Graphs

ones, $\mathcal{I} = \emptyset$, mean over 3 instances

Specifications					Iter	cpu	Bounds			Residuals	
imax	*k*	*n*	*p*	*l*			low	up	rel-gap	prim.	dual
5	6	19.0	0.49	0	333.33	0.89	38.0	38.33	0.01	4.15e-03	6.18e-03
6	7	24.67	0.44	0	500.0	3.03	60.0	61.67	0.02	4.86e-03	8.74e-03
7	8	31.0	0.37	0	966.67	9.53	68.33	71.0	0.04	8.44e-04	3.74e-04
8	9	40.0	0.31	0	833.33	22.75	100.33	110.67	0.09	1.43e-03	6.92e-04
9	10	50.33	0.23	0	1100.0	75.26	119.67	132.33	0.09	1.53e-03	6.81e-04

Numerics cont... Random Graphs

$k \notin \mathcal{I} \neq \emptyset$, mean over 4 instances

Specifications					Iters	cpu	Bounds			Residuals	
imax	k	n	p	l			lower	upper	rel-gap	primal	dual
5	6	16.25	0.51	1.50	450.00	1.02	22.25	23.00	0.03	2.36e-03	1.64e-03
6	7	17.00	0.43	3.25	325.00	1.18	23.00	23.25	0.00	3.75e-02	5.90e-02
7	8	21.00	0.38	3.50	625.00	4.98	34.50	36.00	0.02	3.66e-03	1.95e-03
8	9	21.75	0.30	5.00	400.00	3.36	20.75	21.25	0.01	8.37e-02	9.51e-02
9	10	38.00	0.23	3.25	775.00	25.84	55.25	63.50	0.11	3.26e-03	1.37e-03

Numerics Cont... Random Graphs

$k \in \mathcal{I} \neq \mathcal{K}$, mean 5 instances

Specifications					Iters	cpu	Bounds			Residuals	
imax	*k*	*n*	*p*	*l*			lower	upper	rel-gap	primal	dual
5	6	13.60	0.49	2.80	160.00	0.33	22.60	22.60	0.00	2.55e-02	3.02e-02
6	7	18.00	0.42	3.40	460.00	1.99	37.80	39.00	0.02	5.66e-02	7.10e-02
7	8	22.20	0.39	3.80	560.00	3.96	57.80	60.20	0.02	1.04e-02	1.19e-02
8	9	22.60	0.30	5.20	540.00	4.92	37.20	38.00	0.01	3.48e-02	4.29e-02
9	10	31.00	0.23	4.80	700.00	16.78	61.80	68.00	0.06	1.44e-02	1.01e-02

$\mathcal{I} = \mathcal{K}$, mean 6 instances

Specifications				Iters	Time (cpu)	Bounds			Residuals	
k	*n*	*p*	*l*			lower	upper	rel-gap	primal	dual
6	6.00	0.59	6.00	100.00	0.06	4.67	4.67	0.00	5.12e-03	5.10e-03
7	7.00	0.48	7.00	100.00	0.08	5.67	5.67	0.00	8.66e-02	1.27e-01
8	8.00	0.41	8.00	150.00	0.18	7.17	7.17	0.00	2.64e-01	1.68e-01
9	9.00	0.34	9.00	233.33	0.37	7.83	8.00	0.03	1.88e-01	3.99e-02
10	10.00	0.25	10.00	266.67	0.56	7.50	7.50	0.00	6.28e-02	8.71e-02

Numerics Cont...

Table: Comparisons on the bounds for MC and bounds for the cardinality of separators

Name	n	$\|E\|$	m_1	m_2	m_3	lower (MC by SDP_4)	upper (MC by SDP_4)	lower (MC by DNN-final)	upper (MC by DNN-final)	lower (Separator by SDP_4)	upper (Separator by SDP_4)	lower (Separator by DNN-final)	upper (Separator by DNN-final)
Example 1	93	470	42	41	10	0.07	1	0	1	11	11	11	11
bcspwr03	118	179	58	57	3	0.56	1	0	2	4	5	4	5
Smallmesh	136	354	65	66	5	0.13	1	0	1	6	6	6	6
can-144	144	576	70	70	4	0.90	6	0	6	5	6	5	8
can-161	161	608	73	72	16	0.31	2	0	2	17	18	17	18
can-229	229	774	107	107	15	0.40	6	0	6	16	19	16	19
gridt(15)	120	315	56	56	8	0.29	4	0	4	9	11	9	12
gridt(17)	153	408	72	72	9	0.17	4	0	4	10	13	10	13
grid3dt(5)	125	604	54	53	18	0.54	2	0	4	19	19	19	22
grid3dt(6)	216	1115	95	95	26	0.28	4	0	4	27	30	27	31
grid3dt(7)	343	1854	159	158	26	0.60	22	0	27	27	37	27	44

Numerics for SCP, Small, Medium Proteins

Table 3 Results on small proteins

Protein	n_0	p	run time (sec)		dual SDP optval		objval in IQP		relative diff		relative gap	
			SCPCP	[6]	SCPCP	[6]	SCPCP	[6]	SCPCP	[6]	SCPCP	[6]
1AAC	117	85	6.58	296.06	-206.33	-206.33	-206.33	-206.33	5.75E-11	1.72E-05	1.30E-09	4.21E-04
1AHO	108	54	7.97	364.73	33.53	33.53	33.53	33.53	8.44E-11	4.95E-05	2.45E-09	4.68E-04
1BRF	130	45	14.96	977.08	-31.11	-31.11	-31.11	-31.11	3.92E-11	2.27E-05	3.08E-09	1.24E-04
1CC7	160	66	28.60	1059.06	-63.76	-2.30E+07	-63.76	3.73E+04	1.13E-11	2.01	1.27E-09	1.11
1CKU	115	60	5.46	815.18	113.83	113.83	113.83	113.83	7.17E-11	4.79E-05	3.42E-09	1.13E-04
1CRN	65	37	12.76	46.42	-14.87	-14.87	-14.87	-14.87	1.64E-12	3.05E-05	2.20E-10	3.66E-04
1CTJ	153	61	16.15	777.31	-129.53	-6.69E+06	-129.53	174.65	2.98E-11	2.00	2.29E-09	1.07
1D4T	188	89	41.32	2775.34	-173.03	-2.96E+07	-173.03	291.13	3.88E-11	2.00	1.35E-09	1.20
1IGD	82	50	5.51	189.04	-69.25	-69.25	-69.25	-69.25	4.79E-10	2.74E-06	5.76E-09	3.39E-05
1PLC	129	82	14.32	1766.03	-1.50	-1.50	-1.50	-1.50	1.28E-11	7.28E-04	4.60E-10	1.09E-03
1VFY	134	63	23.49	1765.36	-90.09	-90.09	-90.09	-90.09	1.67E-11	-1.11E-05	9.15E-10	3.79E-05
4RXN	98	48	18.44	366.48	-21.65	-21.65	-21.65	-21.65	1.48E-11	2.62E-05	4.19E-10	6.67E-05

Table 4 Results on medium-sized proteins

Protein	n_0	p	run time (min)		dual SDP optval		objval in IQP		relative diff		relative gap	
			SCPCP	[6]	SCPCP	[6]	SCPCP	[6]	SCPCP	[6]	SCPCP	[6]
1B9O	265	112	0.64	254.85	-140.24	-5.63E+07	-140.24	1.91E+06	1.19E-11	2.14	1.45E-09	1.24
1C5E	200	71	2.59	70.63	-131.75	-6.46E+04	-131.75	148.82	4.93E-11	2.01	5.02E-09	1.00
1C9O	207	53	2.15	66.50	-83.55	-1.88E+06	-83.55	1628.10	3.35E-12	2.00	2.77E-10	1.02
1CZP	237	83	1.90	143.95	-37.88	-2.26E+04	-37.88	1254.42	8.30E-11	2.24	1.03E-08	1.00
1MFM	216	118	0.19	102.11	-201.29	-7.36E+07	-201.29	1369.92	2.01E-11	2.00	1.24E-09	1.09
1QQ4	365	143	5.70	-	-102.40	-	-102.40	-	6.49E-11	-	2.27E-08	-
1QTN	302	134	5.04	-	-178.77	-	-178.77	-	2.24E-11	-	4.12E-09	-
1QU9	287	101	7.55	-	-124.96	-	-124.96	-	1.80E-11	-	5.52E-09	-

Numerics for SCP, Large Proteins

Table 5 Results on large proteins (SCPCP only)

Protein	n_0	p	run time (hr)	dual SDP optval	Objval in IQP	rel. diff	rel. gap	numcut	# iter	Final # cuts
1CEX	435	146	0.08	140.20	140.20	1.26E-11	5.57E-09	40	9	485
1CZ9	615	111	3.96	497.46	497.46	2.98E-13	6.37E-10	60	25	1997
1QJ4	545	221	0.15	-286.83	-286.83	5.31E-12	1.14E-09	60	14	1027
1RCF	581	142	0.85	-191.54	-191.54	3.71E-12	1.15E-08	60	17	1305
2PTH	930	151	29.65	-159.41	-159.41	8.69E-09	7.63E-06	120	34	7247
5P21	464	144	0.31	-135.75	-135.75	1.39E-12	7.33E-10	40	16	822

Thanks for your attention!

**Hard Combinatorial Problems,
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and
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Henry Wolkowicz
Dept. Comb. and Opt., University of Waterloo, Canada

Monday, Aug. 2, 2021, 9:00-10:00 AM, EDT

7th Annual LLU Algorithm Workshop