Online generation via offline selection
- Low dimensional linear cuts from QP SDP relaxation -

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https://www.dropbox.com/s/sfpiy9godzqo2t3/preprint.pdf?dl=0

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Deterministically solving non-convex QP

QP :

$$\min_x x^T Qx + c^T x$$
$$\text{s.t. } Ax \le b,$$
$$x \in [0,1]^N$$

Prior work: Branch & Cut with relaxations

- **RLT** McCormick + ext., e.g. triangle ineq. Bonami et al. [2016]
- **SDP/SOCP/Convex** Dong [2016], Saxena et al. [2011], Buchheim and Wiegele [2013], Zheng et al. [2011], Bao et al. [2011], Anstreicher [2009], Chen and Burer [2012]
- **LP** relaxation of SDP (typically high dimensional) e.g. Qualizza et al. [2012], Sherali and Fraticelli [2002]
- **Edge-concave** Bao et al. [2009], Misener and Floudas [2012]

This work: Off-line (learned) selection of low-dim. LP cuts from SDP

- Develop **online strong low dimensional linear cuts**;
- **Offline cut selection** via **neural net estimator trained "a priori"**;
- **Cheaply outer-approximate SDP** esp. in combination with other low-dim cuts (RLT, triangle, edge-concave, Boolean quadric polytope).

SDP & RLT relaxations

(Anstreicher, *J Glob Optim*, 2009)

$$\min_x \quad x^T Q x + c^T x$$
$$Ax \leq b,$$
$$x \in [0,1]^N$$

- $X_{ij} = X_{ji}$,
- $Q \bullet X$ is the matrix inner product $Q \bullet X = \sum_{i,j=1}^N Q_{ij} \cdot X_{ij}$,
- SDP $\equiv$ Semidefinite programming,
- RLT $\equiv$ Reformulation linearisation technique.

SDP & RLT relaxations

(Anstreicher, *J Glob Optim*, 2009)

$$\begin{aligned} \min_x \quad & Q \bullet X + c^T x \\ & Ax \leq b, \\ & X = xx^T \\ & x \in [0,1]^N \\ & X \in [0,1]^{N \times N} \end{aligned}$$

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SDP & RLT relaxations

(Anstreicher, *J Glob Optim*, 2009)

$$
\begin{aligned}
\min_x \quad & Q \bullet X + c^T x \\
& Ax \le b, \\
& X = xx^T \\
& x \in [0,1]^N \\
& X \in [0,1]^{N \times N}
\end{aligned}
\quad \Rightarrow \quad
\begin{aligned}
\min_x \quad & Q \bullet X + c^T x \\
& Ax \le b, \\
& \mathbf{X} \succeq \mathbf{xx^T} && \textbf{SDP relaxation} \\
& \mathbf{X_{ii}} \le \mathbf{x_i} \\
& X_{ij} - x_i - x_j \ge -1 \\
& X_{ij} - x_i \le 0 && \text{RLT relaxation} \\
& X_{ij} - x_j \le 0 \\
& x \in [0,1]^N \\
& X \in [0,1]^{N \times N}
\end{aligned}
$$

- $X_{ij} = X_{ji}$,
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SDP & RLT relaxations

(Anstreicher, *J Glob Optim*, 2009)

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SDP relaxation (red constraints)

RLT relaxation (blue constraints)

- $X_{ij} = X_{ji}$,
- $Q \bullet X$ is the matrix inner product $Q \bullet X = \sum_{i,j=1}^{N} Q_{ij} \cdot X_{ij}$,
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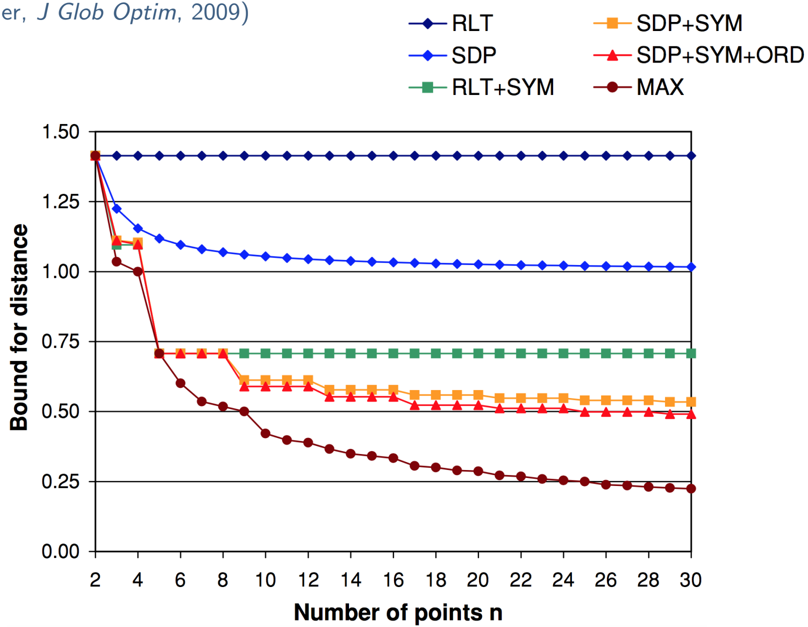
SDP & RLT relaxations: Point Packing

(Anstreicher, *J Glob Optim*, 2009)



Schur's complement & Decomposition for SDP relaxations

Schur's complement

SDP Relaxation $X = xx^T \Rightarrow \text{relax} \Rightarrow X \succeq xx^T$

Schur's complement $X \succeq xx^T \iff \begin{bmatrix} 1 & x^T \\ x & X \end{bmatrix} \succeq 0$

Key Idea Consider smaller subsets

We have $X = xx^T$, so $X_S = x_S\, x_S^T$ for all $S \subset \overline{1, N}$, e.g.

$$\begin{bmatrix} 1 & x_1 & x_2 & x_3 & x_4 \\ x_1 & X_{11} & X_{12} & X_{13} & X_{14} \\ x_2 & X_{21} & X_{22} & X_{23} & X_{24} \\ x_3 & X_{31} & X_{32} & X_{33} & X_{34} \\ x_4 & X_{41} & X_{42} & X_{43} & X_{44} \end{bmatrix} \succeq 0 \implies \begin{bmatrix} 1 & x_1 & x_2 & x_3 \\ x_1 & X_{11} & X_{12} & X_{13} \\ x_2 & X_{21} & X_{22} & X_{23} \\ x_3 & X_{31} & X_{32} & X_{33} \end{bmatrix} \succeq 0$$

Sum-additive objective decomposition

Recall Power set $\mathcal{P}_n$

If finite set S has $|S| = n$ elements, then S has $|\mathcal{P}_n| = 2^n$ subsets.

$$\begin{aligned} \min_x \quad & Q \bullet X + c^T x \\ & Ax \leq b, \\ & X = xx^T \\ & x \in [0,1]^N \\ & X \in [0,1]^{N \times N} \end{aligned} \quad \Longrightarrow \quad \begin{aligned} \min_x \quad & \sum_{\forall S \in \mathcal{P}_n} Q'_S \bullet X_S + c^T x \\ & Ax \leq b, \\ & X = xx^T \\ & x \in [0,1]^N \\ & X \in [0,1]^{N \times N} \end{aligned}$$

Initial RLT relaxation

$$\begin{aligned} \min_x \quad & Q \bullet X + c^T x \\ & Ax \le b, \\ & X = xx^T \\ & x \in [0,1]^N \\ & X \in [0,1]^{N \times N} \end{aligned} \quad \Rightarrow \quad \begin{aligned} \min_x \quad & Q \bullet X + c^T x \\ & Ax \le b, \\ & X_{ij} - x_i - x_j \ge -1 \quad \forall\, i,j \\ & X_{ij} - x_i \le 0 \quad \forall\, i,j \\ & X_{ij} - x_j \le 0 \quad \forall\, i,j \\ & X_{ij} = X_{ji} \quad \forall\, i,j \\ & x \in [0,1]^N \\ & X \in [0,1]^{N \times N} \end{aligned} \quad \Rightarrow \tilde{x}, \tilde{X}$$

Cutting plane motivation

- $\tilde{x}$ is feasible in the space of the original QP,
- For nonconvex QP, $\tilde{X}$ may be infeasible in the original QP,
- I find LP solvers easier to use than SDP solvers,
- As in MIP & SAT, may want low-dimensional cutting planes.

A decomposition of the SDP relaxation for QP

(1) QP SDP relaxation

$$\min_{x,X} Q \cdot X + c^T x$$
$$\text{s.t. } Ax \le b,$$
$$\begin{bmatrix} 1 & x^T \\ x & X \end{bmatrix} \succeq 0,$$
$$x \in [0,1]^N, \; X_{ii} \le x_i \; \forall i$$

(2) QP SDP relaxation at given point $\tilde{x}$

$$\min_X f(X|\tilde{x}) = Q \cdot X$$
$$\text{s.t. } \begin{bmatrix} 1 & \tilde{x}^T \\ \tilde{x} & X \end{bmatrix} \succeq 0, \; X_{ii} \le \tilde{x}_i \; \forall i$$

(3) Relaxed QP SDP relaxation at given $\tilde{x}$

$$\min_X \sum_{\forall S \in \mathcal{P}_n} f_S(X_S|\tilde{x}_S)$$
$$\text{s.t. } \begin{bmatrix} 1 & \tilde{x}_S^T \\ \tilde{x}_S & X_S \end{bmatrix} \succeq 0 \; \forall S \in \mathcal{P}_n, \; X_{ii} \le \tilde{x}_i \; \forall i,$$

where $\mathcal{P}_n = \{S \subset \overline{1,N}, \; |S| = n \le N\}$ (*) and,

$$f(X|\tilde{x}) = Q \cdot X = \sum_{\forall S \in \mathcal{P}_n} Q_S \cdot X_S = \sum_{\forall S \in \mathcal{P}_n} f_S(X_S|\tilde{x}_S).$$

(4) nD-SDP sub-problems
Parameters: $n, S, Q_S, \tilde{x}_S$

$$\forall S \in \mathcal{P}_n \begin{cases} f_S^*(X_S^*|\tilde{x}_S) = \min_{X_S} Q_S \cdot X_S \\ \text{s.t. } \begin{bmatrix} 1 & \tilde{x}_S^T \\ \tilde{x}_S & X_S \end{bmatrix} \succeq 0, \quad X_{ii} \le \tilde{x}_i \; \forall i \in S \end{cases}$$

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$$\min_{x,X} Q \cdot X + c^T x$$

$$\text{s.t.} \quad Ax \leq b,$$

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$$\min_X f(X|\tilde{x}) = Q \cdot X$$

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(*) We take $n = 3, 4, 5$ in our experiments.

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$$\min_{X} f(X|\tilde{x}) = Q \cdot X$$

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(4) nD-SDP sub-problems

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Cut selection from nD-SDP sub-problems at given $\tilde{x}$

Generate outer-approximate hyperplanes for each nD-SDP

$$\forall S \in \mathcal{P}_n : \quad f_S(X_S^* | \tilde{x}_S) = \min_{X_S} Q_S \cdot X_S,$$
$$\text{s.t.} \begin{bmatrix} 1 & \tilde{x}_S^T \\ \tilde{x}_S & X_S \end{bmatrix} \succeq 0, \quad X_{ii} \leq \tilde{x}_i \; \forall i \in S$$

(Given n, S, parametric on $Q_S, \tilde{x}_S$)

Combinatorial explosion!

sub-problems $= \binom{N}{n}$, need **quick optimal selection of a few sub-problems** for generating hyperplanes

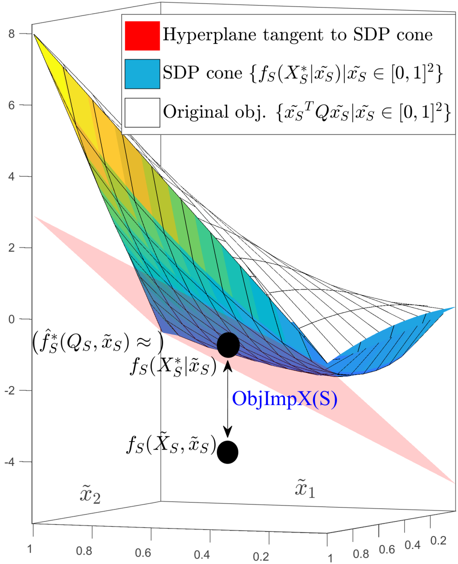
Selection of nD-SDP sub-problems to cut

- Assume current sol. $\tilde{X}, \tilde{x}$ with S sub-problem objective $f_S(\tilde{X}_S, \tilde{x}_S)$
- Order/select top S (to cut off $\tilde{X}, \tilde{x}$ via $\tilde{X}_S, \tilde{x}_S$) by estimated objective improvement on X, ObjImpX(S):

$$\Big(f_S(X_S^* | \tilde{x}_S) - f_S(\tilde{X}_S, \tilde{x}_S) \approx \Big)$$
$$\hat{f}_S^*(Q_S, \tilde{x}_S) - f_S(\tilde{X}_S, \tilde{x}_S) = \hat{f}_S^*(Q_S, \tilde{x}_S) - Q_S \cdot \tilde{X}_S, \qquad \text{(ObjImpX(S))}$$

where $\hat{f}_S^*(Q_S, \tilde{x}_S)$ is a **fast estimator** of $f_S^*(\tilde{x}_S, X_S^*)$.

Generating cutting hyperplanes at given $\tilde{X}_S, \tilde{x}_S$ for one nD-SDP sub-problem



Generating hyperplanes

- Could generate separating **hyperplane tangent** to SDP cone.
- **In practice**, generate cuts from **negative eigenvalues**, Qualizza et al. [2012]:

$$v_k^T \begin{bmatrix} 1 & \tilde{x}_S^T \\ \tilde{x}_S & X_S \end{bmatrix} v_k = $$
$$= v_k^T \lambda_k v_k = \lambda_k < 0.$$

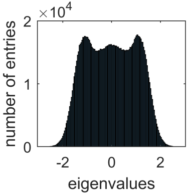
Data for learning estimator $\hat{f}_S^*(Q_S, \tilde{x}_S)$

Estimator only as good as data is sampled

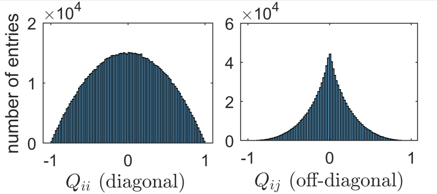
- Critical that sample space $\{Q_S, \tilde{x}_S\}$ is **uniform in important features** for any learner to generalize well
- Features: $\tilde{x}_S$ (positioning), eigenvalues $\{\lambda_i\}$ of Q_S (positive definiteness)

Data sampling

- Uniform $\tilde{x}_S \in [0,1]^n$
- ~~Uniform Q_S elements~~



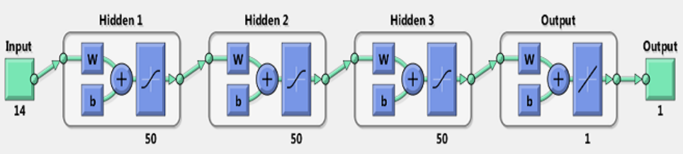
- Uniform $\{\lambda_i\}$ and orthonormal basis



Neural network as estimator $\hat{f}^*_S(Q_S, \tilde{x}_S)$

$Q_S \rightarrow$

$\tilde{x}_s \rightarrow$



$= \hat{f}^*_S(Q_S, \tilde{x}_S)$

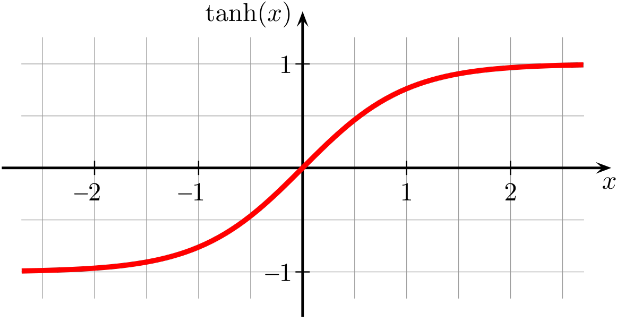
Why neural nets?

- $\hat{f}^*_S$ is a **nonlinear regression** mapping (collection of convex surfaces)
- Neural nets (NN): regression via **trained hidden layers**, no need to **specify model**
- Flexible model + lots of well sampled data $\approx$ **low variance and bias**

Architecture (for 3-5D cases)

- 3-4 hidden layers with 50-64 neurons
- *tanh* activation (well-scaled with our data) in hidden layers
- Trained by 5-fold cross-validation on 1M data pts. with scaled conjugate gradient
- Early stop on low gradient (10^{-5})

Engineering Non-linear activation function



Non-linear activation function in the hidden layers

Hyperbolic tangent (*tanh*) vs. Rectified linear unit (ReLU):

- *tanh* faster to train,
- *tanh* has a bounded output of $[-1, 1]$,
- *tanh* has a significantly positive derivative on the domain $[-4, 4]$,
- *tanh* is symmetric around 0.

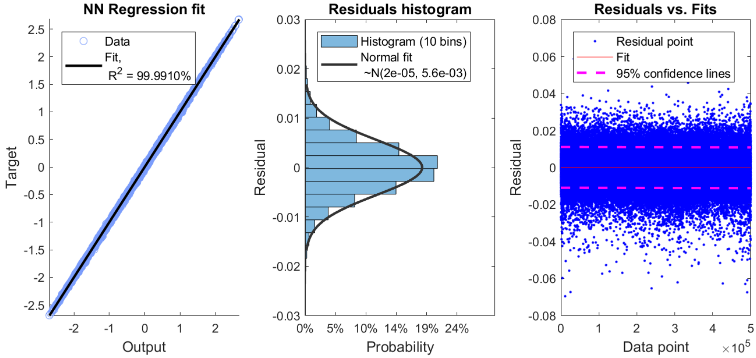
Are the domain and co-domain bounds okay?

Lemma. *If all eigenvalues of a square matrix M are bounded within $[-m, m]$ then any element in M is bounded within $[-m, m]$.*

Let $M \in \mathbb{R}^{n\times n}$ with eigenvalues and eigenvectors λ_i and v_i for $\forall i \in \overline{1, n}$, and let v_{ij} be the j-th element of v_i. Then the absolute value of element M_{ij} on the i-th row and j-th column can be expressed as:

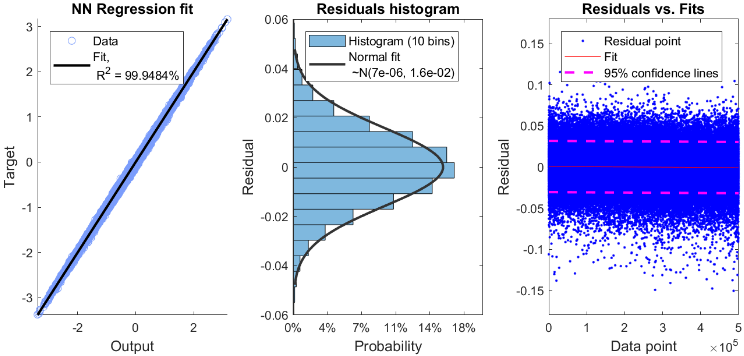
$$\begin{aligned}|M_{ij}| &= \left|\sum_{k\in\overline{1,n}} v_{ki} v_{jk} \lambda_k\right| \\ &\leq \sum_{k\in\overline{1,n}} |v_{ki} v_{jk}| \cdot |\lambda_k| \\ &\leq \sum_{k\in\overline{1,n}} ((v_{ki}^2 + v_{jk}^2)/2) \cdot |\lambda_k| \\ &\leq \sum_{k\in\overline{1,n}} ((v_{ki}^2 + v_{jk}^2)/2) m = m\end{aligned}$$

Neural network training (3D case) - Results on .5M test set



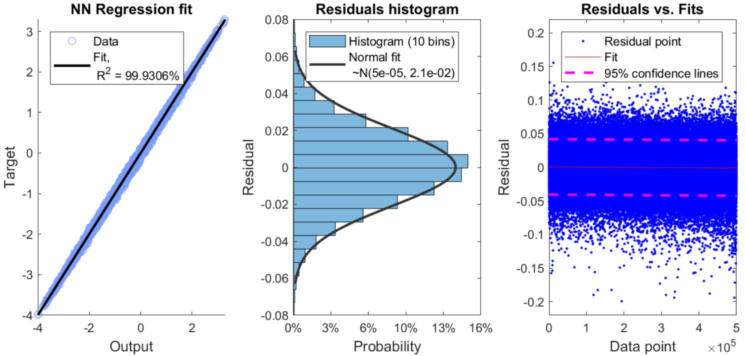
3D-SDP trained NN (9 inputs layer + 3 hidden layers x 50 neurons)

Neural network training (4D case) - Results on .5M test set



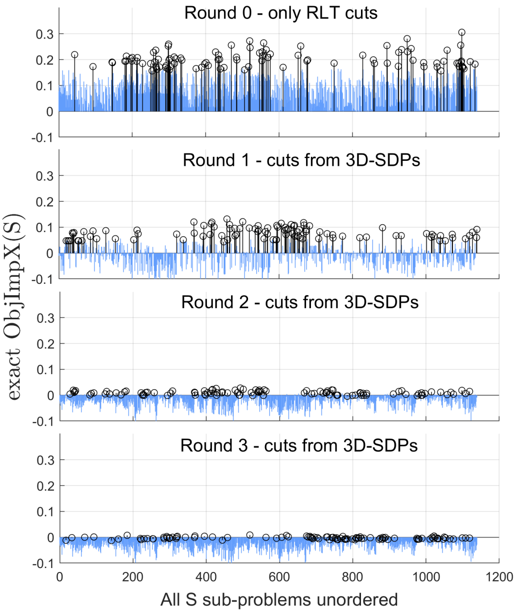
4D-SDP trained NN (14 inputs layer + 3 hidden layers x 64 neurons)

Neural network training (5D case) - Results on .5M test set



5D-SDP trained NN (20 inputs layer + 4 hidden layers x 64 neurons)

Cut selection in practice



BoxQP *spar020-100-1*

- 4 rounds of cuts, $n = 3$, 100 S sub-problems selected by $ObjImpX(S)$ (black lines)

Better bound by few cuts

- After each round, overall bound improving as $ObjImpX(S) \searrow$ across S

Cut selection in practice

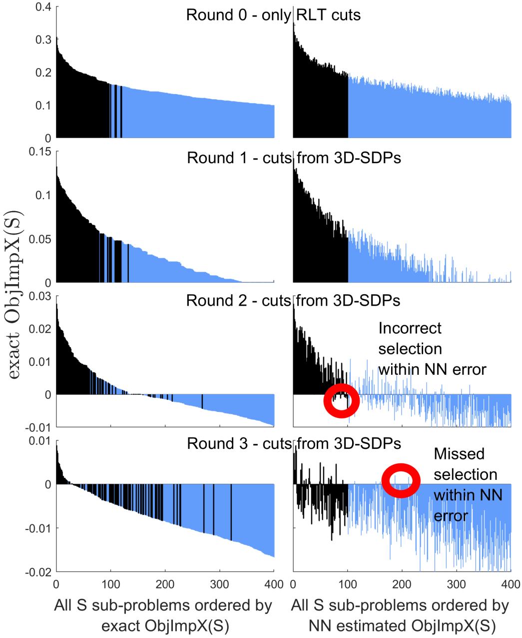
BoxQP *spar020-100-1*

- 4 rounds of cuts, $n = 3$, 100 S sub-problems selected by $ObjImpX(S)$ (black lines)

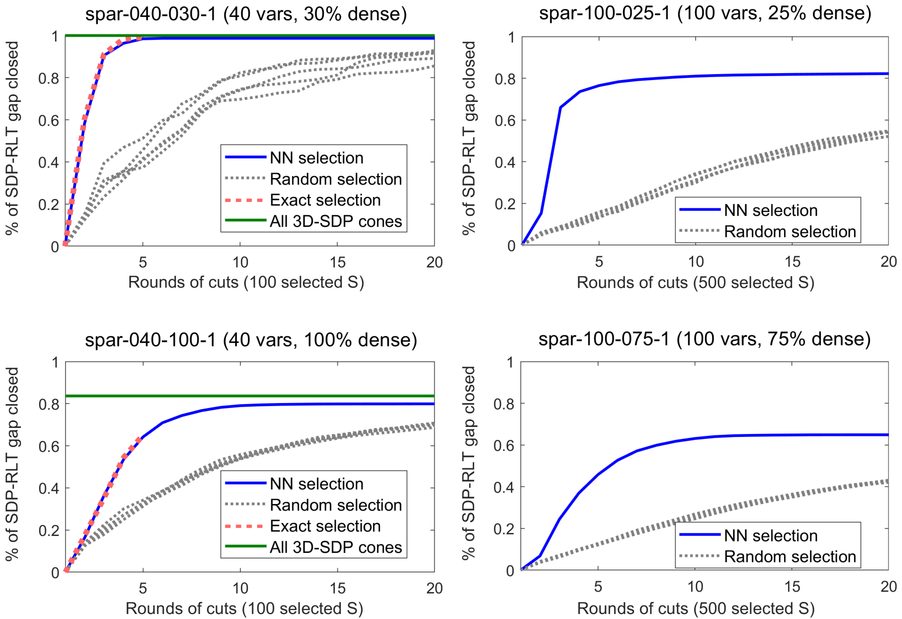
Limits - NN error

After a few rounds, as $ObjImpX(S) \searrow$ NN error:

- Incorrect selection of S where $ObjImpX(S) < 0$
- Missed selection of S where $ObjImpX(S) > 0$



Results for different problem sizes/densities ($n = 3$)



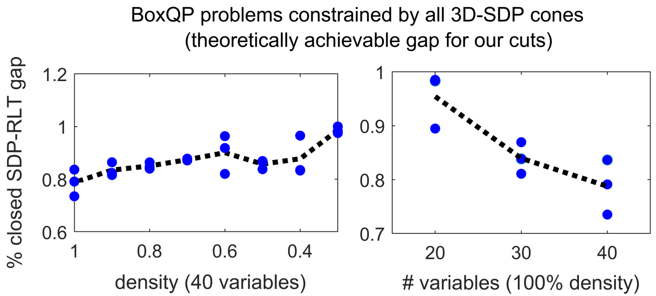
Conclusion

Pluses

- Offline cut selection
- Good bounds with few low-dimensional linear cuts
- Easily integrate SDP-based linear cuts with other cut classes in Branch&Cut

Minuses

- Weaker bounds then full SDP or convex-based relaxations
- Best complemented by other linear cutting planes (e.g. RLT-based)
- Limited to low-dimensionality cuts



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