# SDPNAL+: A MATLAB software package for large-scale SDPs with a user-friendly interface

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#### Outline

- SDP and SDP+ (variable is positive semidefinite and bounded)
- Some examples of SDP+
- User-friendly interface
- Phase I: An inexact symmetric Gauss-Seidel (sGS) ADMM for SDP+
- An sGS decomposition theorem for convex composite QP
- Phase II: An augmented Lagrangian method (ALM) for SDP+
- A semismooth Newton-CG (SNCG) method for solving ALM subproblems
- SDPNAL+: practical implementation of the 2 phase method
- Numerical experiments

## SDP and SDP+ problems

 $\mathbb{S}^n_+=$  cone of positive semidefinite matrices. Write  $X\succeq 0$  if  $X\in \mathbb{S}^n_+.$ 

(SDP) 
$$\min \{ \langle C, X \rangle \mid \mathcal{A}(X) = b, X \in \mathbb{S}_+^n \}$$

where  $C \in \mathbb{S}^n$ ,  $b \in \mathbb{R}^m$  are given data;  $\mathcal{A} : \mathbb{S}^n \to \mathbb{R}^m$  is a linear map.

$$(\mathsf{SDP+}) \quad \min \left\{ \langle C, \, X \rangle \mid \mathcal{A}(X) = b, \, \, X \in \mathbb{S}^n_+, \, \, X \in \mathcal{N} \right\}$$

where  $\mathcal{N}=\{X\in\mathbb{S}^n\mid L\leq X\leq U\}$  and L,U are given bounds (entries allow to take  $-\infty$ ,  $\infty$  respectively).

Important case:  $\mathcal{N}=\{X\in\mathbb{S}^n\mid X\geq 0\}$ , i.e., DNN (doubly nonnegative) SDP.

(SDP) is solvable by powerful interior-point methods if n and m are not too large, say,  $n \le 2000$ ,  $m \le 10,000$ .

 $m \ {\rm large} \Rightarrow m \times m \ {\rm dense}$  "Hessian" matrix cannot be stored explicitly. For  $m=10^5$ , needs 100GB RAM memory!

Current research interests focus on  $n \le 5000$  but  $m \gg 10,000$ .

### More general SDP+

SDPNAL was developed around 2008/09 for (SDP).

In 2012/13, it was extended to SDPNAL+ for (SDP+) directly without introducing extra equality constraints X=Y to convert  $X\in\mathbb{S}^n_+\cap\mathcal{N}$  to  $X\in\mathbb{S}^n_+$  and  $Y\in\mathcal{N}$ .

Now our solver SDPNAL+ can solve general SDP problems:

(genSDP) 
$$\min \quad \sum_{i=1}^N \langle C_i, X_i \rangle$$
  
s.t.  $\sum_{i=1}^N \mathcal{A}_i(X_i) = b$  (equalities) 
$$l \leq \sum_{i=1}^N \mathcal{B}_i(X_i) \leq u \quad \text{(inequalities)}$$

$$X_i \in \mathbb{K}_i \quad \text{(cone)}, \quad X_i \in \mathcal{N}_i \quad \text{(bounds)}, \quad i = 1:N$$

where  $\mathbb{K}_i$  is either a PSD cone or nonnegative orthant. Currently extending  $\mathbb{K}_i$  to other cones such as SOCP.

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## Large scale SDP and SDP+: a brief history

- Parallel IPM [Benson, Borchers, Fujisawa, ... 03-present]
- First-order gradient methods on NLP formulation (low accuracy)
   [Burer-Monteiro 03]
- Inexact IPM [Kojima, Toh 04]
- Gen. Lag. method on barrier-penalized dual [Kocvara-Stingl 03]
- ALM on primal SDP from relaxation of lift-and-project scheme [Burer-Vandenbussche 06]
- Boundary-point method: BCD-ALM on dual [Rendl et al. 06] Reg. methods for SDP  $\equiv$  ADMM on dual [Malick-Povh-Rendl 09]
- SDPNAL: ADMM+SNCG-ALM on dual [Zhao-Sun-Toh 10]
- SDPAD: ADMM on dual [Wen et al. 10] (used SDPNAL template)
- 2EBD: hybrid proximal extra-gradient method on primal [Monteiro et al. 13] (used SDPNAL template)
- ADMM+: convergent sGS-ADMM on SDP+ [Sun-Toh-Yang 15]
- SDPNAL+: SNCG-ALM on SDP+ [Yang-Sun-Toh 15]

#### Correlation matrix and clustering problems

In nearest correlation matrix problem, given data matrix  $U \in \mathbb{S}^n$ , we want to solve

$$(\mathsf{NCM}) \quad \min_X \left\{ \frac{1}{2} \| H \circ (X - U) \|_1 \ | \ \mathrm{Diag}(X) = \mathbf{1}, \ X \succeq 0 \right\} \quad \bullet^{\mathsf{NCM}}$$

where  $H \in \mathbb{S}^n$  has nonnegative entries and " $\circ$ " is the Hardamard product.

In clustering, given data vectors  $\{p_i\}_{i=1}^n$ , the goal is to cluster them into k clusters. A possible model [Peng-Wei 07] is:

$$\min \left\{ \langle D,\, X\rangle \mid \langle I,\, X\rangle = k, \; X\mathbf{1} = \mathbf{1}, \; X \in \mathbb{S}^n_+, \; X \geq 0 \right\} \quad \text{ $\bullet$ Clustering}$$

where  $D_{ij} = ||p_i - p_j||^2$ .

Note: D can also be other affinity matrix.

## Maximum stable set problem a graph $G = (V, \mathcal{E})$

A stable set S is subset of V such that no vertices in S are adjacent. Maximum stable set problem: find S with maximum cardinality. Let

$$x_i = \begin{cases} 1 & \text{if } i \in S \\ 0 & \text{otherwise} \end{cases} \Rightarrow |S| = \sum_{i=1}^n x_i.$$

A common formulation of the max-stable-set problem:

$$\alpha(G) := \max \left\{ |S| = \frac{1}{|S|} \sum_{ij} x_i x_j \mid x_i x_j = 0 \ \forall \ (i,j) \in \mathcal{E}, x \in \{0,1\}^n \right\}$$

$$\downarrow X := x x^T / |S|$$

$$\max \left\{ \langle E, X \rangle \mid X_{ij} = 0 \ \forall \ (i,j) \in \mathcal{E}, \ \langle I, X \rangle = 1 \right\}$$

SDP relaxation:  $X = xx^T/|S| \Rightarrow X \succeq 0$ , get

$$\theta(G) := \max \left\{ \langle E, X \rangle : X_{ij} = 0 \ \forall \ (i, j) \in \mathcal{E}, \ \langle I, X \rangle = 1, \ X \succeq 0 \right\}$$

## Quadratic assignment problem (QAP)

Assign n facilities to n locations [Koopmans and Beckmann (1957)]

$$A = (a_{ij}) \quad \text{where } a_{ij} = \text{flow from facility } i \text{ to facility } j$$
 
$$B = (b_{kl}) \quad \text{where } b_{kl} = \text{ distance from location } k \text{ to location } l$$
 
$$\text{cost of assignment } \pi = \sum_{i=1}^n \sum_{j=1}^n a_{ij} b_{\pi(i)\pi(j)}$$
 
$$\min_{P} \left\{ \langle B \otimes A, \operatorname{vec}(P) \operatorname{vec}(P)^T \rangle \mid P \text{ is } n \times n \text{ permutation matrix} \right\}$$

SDP+ relaxation [Povh and Rendl, 09]:

 $\operatorname{relax} \ \operatorname{vec}(P) \operatorname{vec}(P)^T \ \text{to the} \ n^2 \times n^2 \ \text{variable} \ X \in \mathbb{S}^{n^2}_+ \ \text{and} \ X \geq 0$ 

(QAP) 
$$\min \left\{ \langle B \otimes A, X \rangle \mid \mathcal{A}(X) - b = 0, X \in \mathbb{S}^{n^2}_+, X \ge 0 \right\}$$

where the linear constraints (with m=3n(n+1)/2) encode the condition  $P^TP=I_n,\ P\geq 0.$ 

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## A basic user-friendly interface

Consider the NCM problem.

```
n = 100;
G = randn(n,n);
G = 0.5*(G + G');

model = ccp_model('NCM');
   X = var_sdp(n,n);
   model.add_variable(X);
   model.minimize(l1_norm(X-G));
   model.add_affine_constraint(map_diag(X)==ones(n,1));
model.solve;
```

Consider the  $\theta+$  problem of a graph with adjacency matrix G.

```
▶ theta
```

```
n = 200:
G = triu(sprand(n,n,0.5),1);
[IE, JE] = find(G);
n = length(G);
model = ccp_model('theta');
    X = var_sdp(n,n);
    model.add_variable(X);
    model.maximize(sum(X));
    model.add_affine_constraint(trace(X) == 1);
    model.add_affine_constraint(X(IE, JE) == 0);
    model.add_affine_constraint(X >= 0);
model.solve;
```

```
s.t. -X_{12}^{(1)} + 2X_{22}^{(2)} + 2X_{2}^{(3)} = 4 (equalities)
                  2X_{22}^{(1)} + X_{42}^{(2)} - X_{4}^{(3)} = 3
                  2 < -X_{12}^{(1)} - 2X_{22}^{(2)} + 2X_{2}^{(3)} < 7 (inequalities)
                  X^{(1)} \in \mathbb{S}^6_+, X^{(2)} \in \mathbb{R}^{5 \times 5}, X^{(3)} \in \mathbb{R}^7_+ (cones)
                  0 < X^{(1)} < 10E_6. 0 < X^{(2)} < 8E_5 (bounds)
n1 = 6; n2 = 5; n3 = 7;
M = ccp_model('Example_simple');
X1=var_sdp(n1,n1); X2=var_nn(n2,n2); X3=var_nn(n3);
M.add_variable(X1,X2,X3);
M.minimize(trace(X1) + trace(X2) + sum(X3));
M.add_affine_constraint(-X1(1,2)+2*X2(3,3)+2*X3(2)==4);
M.add_affine_constraint(2*X1(2,3)+X2(4,2)-X3(4) == 3);
M.add_affine_constraint(2 \le -X1(1,2) -2 \times X2(3,3) +2 \times X3(2) \le 7);
M.add_affine_constraint(0 <= X1 <= 10);</pre>
```

min  $\operatorname{trace}(X^{(1)}) + \operatorname{trace}(X^{(2)}) + \operatorname{sum}(X^{(3)})$ 

M.add\_affine\_constraint(X2 <= 8);</pre>

M.solve;

#### Dual SDP+

For simplicity, consider only  $\mathcal{N} = \{X \in \mathbb{S}^n \mid X \geq 0\}$ . Dual of SDP+ and its augmented Lagrangian function are given by:

(D) 
$$\min\{-\langle b, y \rangle + \delta_{\mathbb{S}^n_{\perp}}(S) + \delta_{\mathcal{N}}(Z) \mid \mathcal{A}^*y + S + Z = C\}$$

(a linearly constrained convex problem with 3 blocks of variables);

$$\mathcal{L}_{\sigma}(y,S,Z;X) = -\langle b,y\rangle + \langle \mathcal{A}^*y + S + Z - C,X\rangle$$

$$+ \frac{\sigma}{2} \|\mathcal{A}^*y + S + Z - C\|^2 + \delta_{\mathbb{S}^n_+}(S) + \delta_{\mathcal{N}}(Z)$$
(quadratic in  $(y,S,Z)$  + nonsmooth terms in  $S,Z$ )

KKT conditions:

$$\mathcal{R}_{\mathrm{KKT}}(y,S,Z;X) := \left( \begin{array}{c} AX - b \\ S - \Pi_{\mathbb{S}^n_+}(S - X) \\ Z - \Pi_{\mathcal{N}}(Z - X) \\ \mathcal{A}^*y + S + Z - C \end{array} \right) = \left( \begin{array}{c} 0 \\ 0 \\ 0 \\ 0 \end{array} \right).$$

#### A directly extended ADMM for dual SDP+

Input 
$$(y^0,S^0,Z^0;X^0)$$
. For  $k=0,1,\ldots$ , let  $\widehat{C}^k=C-\sigma^{-1}X^k$  (1a)  $y^{k+1}=\mathrm{argmin}_{y\in\mathbb{R}^m}\mathcal{L}_\sigma(y,S^k,Z^k;X^k)$ 

$$\text{(1b) } \underline{S^{k+1}} = \operatorname{argmin}_{S \in \mathbb{S}^n_+} \mathcal{L}_{\sigma}(y^{k+1}, \underline{S}, Z^k; X^k) = \Pi_{\mathbb{S}^n_+}(\widehat{C}^k - \mathcal{A}^*y^{k+1} - Z^k)$$

$$\text{(2) } Z^{k+1} = \mathop{\rm argmin}_{Z \in \mathcal{N}} \mathcal{L}_{\sigma}(y^{k+1}, S^{k+1}, Z; X^k) \ = \ \Pi_{\mathcal{N}}(\widehat{C}^k - \mathcal{A}^* y^{k+1} - S^{k+1})$$

(3) 
$$X^{k+1}=X^k+\tau\sigma(\mathcal{A}^*y^{k+1}+S^{k+1}+Z^{k+1}-C)$$
, where  $\tau\in(0,\frac{1+\sqrt{5}}{2})$  is the step-length.

Direct extension of 2-block ADMM is not guaranteed to converge [Chen-He-Ye-Yuan, v155, MP 2016]

## A convergent symmetric Gauss-Seidel (sGS) ADMM for dual SDP+

Input  $(y^0, S^0, Z^0; X^0)$ . For k = 0, 1, ..., let  $\widehat{C}^k = C - \sigma^{-1} X^k$ 

But sGS-ADMM is guaranteed to converge!

(1a)  $\widehat{\mathbf{y}}^{k+1} \approx \operatorname{argmin}_{y \in \mathbb{R}^m} \mathcal{L}_{\sigma}(y, S^k, Z^k; X^k)$ 

$$\begin{split} &(\text{1b}) \ S^{k+1} = \text{argmin}_{S \in \mathbb{S}^n_+} \mathcal{L}_\sigma(\widehat{\mathbf{y}}^{k+1}, S, Z^k; X^k) = \Pi_{\mathbb{S}^n_+}(\widehat{C}^k - \mathcal{A}^*\widehat{\mathbf{y}}^{k+1} - Z^k) \\ &(\text{1c}) \left[ y^{k+1} \approx \text{argmin}_{y \in \mathbb{R}^m} \mathcal{L}_\sigma(y, S^{k+1}, Z^k; X^k) \right] \\ &(2) \ Z^{k+1} = \text{argmin}_{Z \in \mathcal{N}} \mathcal{L}_\sigma(y^{k+1}, S^{k+1}, Z; X^k) = \Pi_{\mathcal{N}}(\widehat{C}^k - \mathcal{A}^*y^{k+1} - S^{k+1}) \\ &(3) \ X^{k+1} = X^k + \tau\sigma(\mathcal{A}^*y^{k+1} + S^{k+1} + Z^{k+1} - C) \end{split}$$
 In Step 1, the AL function  $\mathcal{L}_\sigma$  for the block  $(y, S)$  has the form:

 $\mathcal{L}_{\sigma}(y, \mathbf{S}, Z^k; X^k) \equiv \delta_{\mathbb{S}^n_+}(\mathbf{S}) + \frac{\sigma}{2} \|\mathcal{A}^* y + \mathbf{S} + Z^k + \widehat{C}^k\|^2 - \langle b, y \rangle$ 

(1a)–(1c) is equivalent to minimizing  $\mathcal{L}_{\sigma}(y, S) + \mathsf{sGS}$  proximal term.

The steps are based on a sGS decomposition theorem.

(QP in (y, S) + nonsmooth term in S)

#### Global convergence of inexact sGS-ADMM

**Theorem** Suppose the KKT conditions of (SDP+) has a solution. Let  $\{(y^k, S^k, Z^k, X^k)\}$  be the sequence generated by the inexact sGS-ADMM. Then  $\{X^k\}$  converges to an optimal solution of (SDP+) and  $\{(y^k, S^k, Z^k)\}$  converges to an optimal solution of its dual.

- [1] D.F. Sun, K.C. Toh and L.Q. Yang, A convergent 3-block semi-proximal ADMM for conic programming with 4-type constraints, v25, SIOPT 2015.
- [2] X.D. Li, D.F. Sun, K.C. Toh, A Schur complement based semiproximal ADMM for convex ..., v155, MP 2016. Schur-complement-ADMM
- [3] X.D. Li, D.F. Sun, K.C. Toh, QSDPNAL: A two-phase augmented Lagrangian method for convex quadratic SDP, arXiv:1512.08872v1, 2015. Section 2: sGS decomposition theorem, Schur-complement-ADMM = sGS-ADMM
- [4] L. Chen, D.F. Sun, K.C. Toh, An efficient inexact symmetric Gauss-Seidel based majorized ADMM for ..., v161, MP 2017. inexact sGS-ADMM
- [5] X.D. Li, D.F. Sun, K.C. Toh, A block sGS decomposition theorem for convex composite quadratic programming and its applications, arXiv:1703.06629, 2017. sGS-ADMM = Schur-complement-ADMM, sSOR-extension

#### Local convergence of inexact sGS-ADMM

**Theorem** [Han-Sun-Zhang, MOR 2017: exact version] Let  $\Omega_{\rm KKT} \neq \emptyset$  be the KKT solution set. Suppose an error bound condition holds for  $\mathcal{R}_{\rm KKT}$  at an optimal solution  $u^* = (y^*, S^*, Z^*, X^*)$ , i.e,  $\exists \ \eta, r > 0$  s.t.

$$\operatorname{dist}(u, \Omega_{\mathrm{KKT}}) \leq \eta \|\mathcal{R}_{\mathrm{KKT}}(u)\| \quad \forall \ u \in B_r(u^*).$$

Let  $u^k=(y^k,S^k,Z^k,X^k).$  Then  $\exists~\mu\in(0,1)$  depending on  $\eta$  s.t.

$$\operatorname{dist}(u^{k+1},\Omega_{\mathrm{KKT}}) \ \leq \ \mu \operatorname{dist}(u^k,\Omega_{\mathrm{KKT}}) \quad \forall \ k \text{ sufficiently large}.$$

Inexact version can be established via the analysis in [Chen-Sun-Toh, MP 2017] and [Han-Sun-Zhang, MOR 2017].

## Detour: block symmetric Gauss-Seidel (sGS) decomposition

Consider a convex composite QP with 3 blocks:

$$\min \left\{ p(x_1) + h(x) \mid x = (x_1; x_2, x_3) \in \mathbb{R}^{n_1} \times \mathbb{R}^{n_2} \times \mathbb{R}^{n_3} \right\}$$

Convex quadratic function  $h(x) := \frac{1}{2}\langle x, \mathcal{H}x \rangle - \langle b, x \rangle$ 

Closed proper convex fun.  $p: \mathbb{R}^{n_1} \to (-\infty, +\infty]$ , eg  $p(x_1) = \|x_1\|_{\infty}$ 

Write  $\mathcal{H} = \mathcal{U}^* + \mathcal{D} + \mathcal{U}$ ,  $\mathcal{D}$  diagonal blocks,  $\mathcal{U}$  strict upper triangular part. Assume  $\mathcal{D}$  invertible.

Define  $sGS(\mathcal{H}) := \mathcal{UD}^{-1}\mathcal{U}^*$  (symmetric Gauss-Seidel decomp.)

Given  $\bar{x}$ , define

$$x^{+} := \operatorname{argmin}_{x} \left\{ p(x_{1}) + h(x) + \frac{1}{2} \|x - \bar{x}\|_{\operatorname{sGS}(\mathcal{H})}^{2} \right\}$$

Next theorem: can compute  $x^+$  using one sGS cycle!

If  $p(x_1)$  is absent, we get the classical block sGS iteration.

## Detour: block symmetric Gauss-Seidel (sGS) decomposition

## Theorem [Li-Sun-Toh 2015]

It holds that 
$$\mathcal{H} + sGS(\mathcal{H}) = (\mathcal{D} + \mathcal{U})\mathcal{D}^{-1}(\mathcal{D} + \mathcal{U}^*) \succ 0.$$

Backward GS:  $3 \rightarrow 2$ . Compute

$$\begin{split} x_3' &= \operatorname{argmin} \, p(\bar{x}_1) + h(\bar{x}_1, \bar{x}_2, x_3) \; = \; \mathcal{H}_{33}^{-1}(b_3 - \mathcal{H}_{13}^* \bar{x}_1 - \mathcal{H}_{23}^* \bar{x}_2) \\ x_2' &= \operatorname{argmin} \, p(\bar{x}_1) + h(\bar{x}_1, x_2, x_3') \; = \; \mathcal{H}_{22}^{-1}(b_2 - \mathcal{H}_{12}^* \bar{x}_1 - \mathcal{H}_{23} \bar{x}_3') \end{split}$$

Forward GS:  $1 \rightarrow 2 \rightarrow 3$ . Compute

$$\begin{aligned} x_1^+ &= \operatorname{argmin} \ p(x_1) + h(x_1, x_2', x_3') \quad \text{(non-smooth/non-quadratic)} \\ x_2^+ &= \operatorname{argmin} \ p(x_1^+) + h(x_1^+, x_2, x_3') = \mathcal{H}_{22}^{-1}(b_2 - \mathcal{H}_{12}^* x_1^+ - \mathcal{H}_{23} x_3') \\ x_3^+ &= \operatorname{argmin} \ p(x_1^+) + h(x_1^+, x_2^+, x_3) = \mathcal{H}_{33}^{-1}(b_3 - \mathcal{H}_{13}^* x_1^+ - \mathcal{H}_{23}^* x_2^+) \end{aligned}$$

Inexact computation is also allowed! So can use PCG to solve large linear systems.

## Detour: block symmetric Gauss-Seidel (sGS) decomposition

#### Theorem [Li-Sun-Toh 2015]

Backward GS: For  $i = s, \ldots, 2$ , compute

$$x_i' = \mathcal{H}_{ii}^{-1} (b_i + e_i' - \sum_{j=1}^{i-1} \mathcal{H}_{ji}^* \bar{x}_j - \sum_{j=i+1}^s \mathcal{H}_{ij} x_j').$$

Forward GS: For  $i = 2, \ldots, s$ 

$$\begin{array}{rcl} x_1^+ & = & \operatorname{argmin} \ p(x_1) + h(x_1, x_{\geq 2}') - \langle e_1^+, \ x_1 \rangle, \\ \\ x_i^+ & = & \mathcal{H}_{ii}^{-1} (b_i + e_i^+ - \sum_{j=1}^{i-1} \mathcal{H}_{ji}^* x_j^+ - \sum_{j=i+1}^{s} \mathcal{H}_{ij} x_j') \end{array}$$

 $e^+$ , e' are error vectors. In this case,  $x^+$  is the exact solution to a slightly perturbed proximal problem:

$$\begin{split} x^+ := \operatorname{argmin}_x \left\{ p(x_1) + h(x) + \frac{1}{2} \|x - \bar{x}\|_{\operatorname{sGS}(\mathcal{H})}^2 - \langle x, \, \Delta(e', e^+) \rangle \right\} \\ \Delta(e', e^+) = e^+ + \mathcal{U} \mathcal{D}^{-1}(e^+ - e'). \end{split}$$

## Phase II: augmented Lagrangian method (ALM)

#### Adding a large proximal term slows the convergence of sGS-ADMM!

With no proximal term added, we consider the ALM for solving dual  $\ensuremath{\mathsf{SDP}}+.$ 

(1) Compute

$$\begin{split} &(y^{k+1},S^{k+1},Z^{k+1}) \; \approx \; \mathrm{argmin} \Big\{ \mathcal{L}_k(y,S,Z) := \mathcal{L}_{\sigma_k}(y,S,Z;X^k) \Big\} \\ &= \mathrm{argmin} \Big\{ - \langle b,\, y \rangle + \frac{\sigma}{2} \|\mathcal{A}^*y + S + Z + \widehat{C}^k\|^2 + \delta_{\mathbb{S}^n_+}(S) + \delta_{\mathcal{N}}(Z) \Big\} \end{split}$$

(2) Update  $X^{k+1} = X^k + \sigma_k(\mathcal{A}^*y^{k+1} + S^{k+1} + Z^{k+1} - C);$  update  $\sigma_{k+1} \uparrow \sigma_{\infty} \leq \infty.$ 

## Global convergence of ALM

Define  $X^{k+1} = X^k + \sigma_k R_D(y^{k+1}, S^{k+1}, Z^{k+1})$ ,

$$e^{k+1} = \left[ \begin{array}{c} \mathcal{A}X^{k+1} - b \\ X^{k+1} - \Pi_{\mathbb{S}^n_+}(X^{k+1} - S^{k+1}) \\ X^{k+1} - \Pi_{\mathcal{N}^n}(X^{k+1} - Z^{k+1}) \end{array} \right].$$

In Step 1, we use the following easy-to-check stopping conditions:

(A) 
$$\|e^{k+1}\| \le \frac{\epsilon_k^2}{1 + \|(X, y, S, Z)^{k+1}\|} \min\left\{\frac{1}{\sigma_k}, \frac{1}{1 + \|X^{k+1} - X^k\|}\right\}$$
  
(B)  $\|e^{k+1}\| \le \frac{\eta_k^2 \|X^{k+1} - X^k\|^2}{1 + \|(X, y, S, Z)^{k+1}\|} \min\left\{\frac{1}{\sigma_k}, \frac{1}{1 + \|X^{k+1} - X^k\|}\right\}$ 

where  $\{\epsilon_k\}$  and  $\{\delta_k\}$  are nonnegative summable sequences.

**Theorem** [Rockafellar 76] Let  $\Omega_P \neq \emptyset$  be the primal optimal solution set and Slater's condition holds for primal problem (P). Under stopping condition (A), we have  $X^k \to X^*$  and  $(y^{k+1}, S^{k+1}, Z^{k+1})$  converges to a dual optimal solution.

#### Local convergence of ALM

**Theorem** [Cui-Sun-Toh] If in addition, the blue stopping conditions are added, and the essential primal objective function  $P^{\text{obj}}$  satisfies a quadratic growth condition at  $X^*$ , i.e.,  $\exists$  a neighborhood  $\mathcal U$  of  $X^*$  and  $\kappa>0$  s.t.

$$P^{\text{obj}}(X) \ge P^{\text{obj}}(X^*) + \kappa^{-1} \text{dist}^2(X, \Omega_P) \quad \forall \ X \in \mathcal{U}$$

Then for k large, we have

$$\operatorname{dist}(X^{k+1},\Omega_P) \; \leq \; \theta_k \operatorname{dist}(X^k,\Omega_P)$$
 dual feasibility at  $(y^{k+1},S^{k+1},Z^{k+1}) \; \leq \; \tau_k \operatorname{dist}(X^k,\Omega_P)$  dual objective gap at  $(y^{k+1},S^{k+1},Z^{k+1}) \; \leq \; \tau_k' \operatorname{dist}(X^k,\Omega_P)$  where  $\theta_k \approx \frac{\kappa}{\sqrt{\kappa^2 + \sigma_k^2}}, \quad \tau_k \approx \frac{1}{\sigma_k}, \quad \tau_k' \approx \frac{\|X^k\| + \|X^{k+1}\|}{2\sigma_k}$ 

Larger  $\sigma_k$  gives faster convergence, but inner problem is harder to solve.

#### ALM-subproblem

For simplicity, assume  $\mathcal{N} = \mathbb{S}^n$  and hence the variable Z is absent.

$$\begin{split} & \mathrm{argmin}_{y,S} \Big\{ \mathcal{L}_{\sigma}(y, \textcolor{red}{S}) \equiv \delta_{\mathbb{S}^n_+}(\textcolor{red}{S}) + \frac{\sigma}{2} \| \mathcal{A}^* y + \textcolor{red}{S} - \widehat{C}^k \|^2 - \langle b, \, y \rangle \Big\} \\ & \equiv \mathrm{argmin}_y \Big\{ \Phi^k(y) := -\langle b, \, y \rangle + \frac{\sigma}{2} \| \Pi_{\mathbb{S}^n_+}(\mathcal{A}^* y - \widehat{C}^k) \|^2 \Big\} \text{ (project out } \textcolor{red}{S} \text{)} \end{split}$$

Optimality condition of unconstrained subproblem in y is:

$$\nabla \Phi^k(y) = -b + \sigma \mathcal{A} \prod_{\mathbb{S}^n_+} (\mathcal{A}^* y - \widehat{C}^k) = 0.$$

Solve for solution  $y^{k+1}$  by semismooth Newton-CG (SNCG) method. Then compute  $S^{k+1} = \prod_{\mathbb{S}^n_+} (\widehat{C}^k - \mathcal{A}^* y^{k+1})$ .

 $\nabla\Phi^k(y)$  is not differentiable, but is strongly semismooth [Sun-Sun, 2002]. Thus SNCG is expected to have at least superlinear convergence.

## A semismooth Newton-CG method (SNCG) for ALM-subproblem

Solve 
$$\nabla \Phi^k(y) = -b + \sigma \mathcal{A} \Pi_{\mathbb{S}^n_+}(U) = 0, \ \ U = \mathcal{A}^* y - \widehat{C}^k.$$

At the current iteration,  $y_l$ , we solve a generalized Newton equation:

$$\mathcal{H}\Delta y \approx \nabla \Phi^k(y_l), \quad \text{where } \mathcal{H}\Delta y = \sigma \mathcal{A} \prod_{S_{\perp}^n}^{\prime}(U)[\mathcal{A}^*\Delta y]$$
 (1)

From eigenvalue decomp:  $U = QDQ^T$  with  $d_1 \ge \cdots \ge d_r \ge 0 > d_{r+1} \ge \cdots \ge d_n$ , we choose

$$\Pi_{\mathbb{S}_{+}^{n}}^{\prime}(U)[M] = Q(\Omega \circ (Q^{T}MQ))Q^{T}, \tag{2}$$

$$\Omega_{ij} = (d_i^+ - d_j^+)/(d_i - d_j)$$
. Let  $\gamma = \{1, \dots, r\}$ ,  $\bar{\gamma} = \{r + 1, \dots, n\}$ ,

$$\Omega = \left[ egin{array}{cc} E_{\gamma\gamma} & \Omega_{\gammaar{\gamma}} \ \Omega_{ar{\gamma}\gamma} & 0 \end{array} 
ight].$$

When problem is primal nondegenerate,  $cond(\mathcal{H})$  is bounded:

$$\operatorname{cond}(\mathcal{H}) \leq \sigma \Theta(1) \operatorname{cond}([\mathcal{A}Q_{\gamma} \otimes Q_{\gamma}, \mathcal{A}Q_{\gamma} \otimes Q_{\bar{\gamma}}])^2$$

## Exploiting second-order structured sparsity

The structure in  $\Omega$  allows for efficient computation of matrix-vector multiply for CG in solving (1). Direct evaluation of

$$Y := \Pi'_{\mathbb{S}^n_+}(U)[M] = Q(\Omega \circ (Q^T M Q))Q^T$$

needs 4 matrix-matrix multiplications =  $8n^3$  operations. But with the structure of  $\Omega$ , can compute Y as follows:

$$Y = H + H^T$$
,  $H = Q_{\gamma} \left[ \frac{1}{2} (UQ_{\gamma}) Q_{\gamma}^T + (\Omega_{\gamma\bar{\gamma}} \circ (UQ_{\bar{\gamma}})) Q_{\bar{\gamma}}^T \right]$ 

where  $U = Q_{\gamma}M$ . The cost is at most  $6rn^2$ .

If  $r \approx n$ , then use

$$Y = Q(E \circ (Q^T M Q))Q^T - Q(\overline{\Omega} \circ (Q^T M Q))Q^T$$
$$= M - Q(\overline{\Omega} \circ (Q^T M Q))Q^T$$

where  $\overline{\Omega}=E-\Omega$  has a similar structure as  $\Omega$  but with a large block of 0. The cost is  $6(n-r)n^2$ .

#### SDPNAL+: a practical implementation of ALM for dual SDP+

Let ADMM+ denote the sGS-ADMM.

- 1. Generate a good starting point to warm-start SNCG-ALM:  $(y^0,S^0,Z^0,X^0,\sigma_0) \leftarrow \mathsf{ADMM} + (\bar{y}^0,\bar{S}^0,\bar{Z}^0,\bar{X}^0,\bar{\sigma}_0)$
- 2. For k = 0, 1, ...

Generate  $(y^{k+1}, S^{k+1}, Z^{k+1})$  in ALM-subproblem via SNCG Compute  $X^{k+1}$  based on  $(y^{k+1}, S^{k+1}, Z^{k+1})$ , update  $\sigma_{k+1}$  If progress of SNCG-ALM is slow,

Rescale data

Let  $(\bar{y}^k, \bar{S}^k, \bar{Z}^k, \bar{X}^k, \bar{\sigma}_k)$  denote rescaled  $(y^k, S^k, Z^k, X^k, \sigma_k)$  Rescaling is chosen such that  $\|\bar{X}^k\| \approx \max\{\|\bar{S}^k\|, \|\bar{Z}^k\|\}$ 

Goto Step 1: Restart with ADMM+ $(\bar{y}^k, \bar{S}^k, \bar{Z}^k, \bar{X}^k, \bar{\sigma}_k)$ 

#### Robustness of SDPNAL+

$$\eta \equiv \frac{\|\mathcal{R}_{KKT}(y^{k+1}, S^{k+1}, Z^{k+1}, X^{k+1})\|}{1 + \|(y^{k+1}, S^{k+1}, Z^{k+1}, X^{k+1})\|} \le 10^{-6}.$$

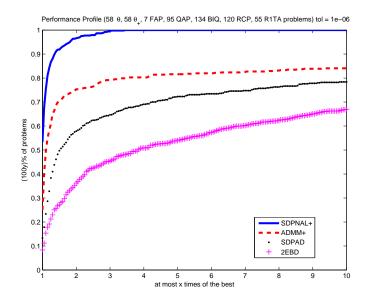
Performance of our SDPNAL+ and ADMM+ versus SDPAD: the directly extended ADMM implemented in [Wen et al.] 2EBD-HPE [Monteiro et al.]

Numbers of problems which are solved to the accuracy  $\eta \leq 10^{-6}$ 

problem set (No.)	SDPNAL+	ADMM+	SDPAD	2EBD
$\theta$ (58)	58	56	53	53
$\theta_+$ (58)	58	58	58	56
FAP (7)	7	7	7	7
QAP (95)	95	39	30	16
BIQ (134)	134	134	134	134
RCP (120)	120	120	114	109
R1TA (55)	55	42	47	18
Total (527)	527	456	443	393

## Performance profile on 527 large SDPs

## Performance profiles of SDPNAL+, ADMM+, SDPAD and 2EBD



#### Numerical results for SDPNAL+

Implemented the algorithms in  $\operatorname{MATLAB}$ .

Runs perform on PC with (12 cores) Intel Xeon CPU E5-2680 @ 2.50 GHz and 128 GB RAM.

Stop SDPAD and 2EBD after 25000 iterations or 20 hours.

Prob	m; n	$\eta$	time (hour:minute)
		SDPAD 2EBD SDPNAL+	
1dc.2048	58368+N; 2048	9.9-7  9.9-7  9.9-7	3:56  2:10  1:08
fap25	2118+N; 2118	9.9-7   9.9-7   9.5-7	3:26  0:54  0:43
nug30	1393+N; 900	1.1-5   1.7-5   9.6-7	2:10  1:46  0:09
tai30a	1393+N; 900	4.6-6   1.3-5   9.9-7	2:34  1:47  0:10
nsym_rd[40,40,40]	672399; 1600	1.5-3   2.0-3   8.6-7	2:48  4:54  0:04
nonsym(14,4)	1.16M; 2744	1.4-2  5.2-3  1.3-7	7:39  14:01  0:20

Results show that it is essential to use **second-order information** and **second-order structured sparsity** to solve hard problems!

## Summary and future work

- We have tested SDPNAL+ on about 520 SDPs from  $\theta, \theta_+$ , QAP, binary QP, rank-1 tensor approximation, etc
- When the problems are primal-dual nondegenerate, SDPNAL+ can efficiently solve large SDPs to high accuracy. SDPAD and 2EDB also performed well, though SDPNAL+ is often much more efficient.
- Many of the tested SDPs are degenerate, but SDPNAL+ can still solve them accurately with  $\eta < 10^{-6}$ . On the other hand, SDPAD and 2EDB were not able to solve many such problems.

#### Currently under development:

- sparse SDPNAL+ so as to handle larger matrix variable when the data has conducive sparsity structure
- 2 a more advanced user-friendly interface

Thank you for your attention!