Large Scale Semidefinite Programming in ConicBundle

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based on joint work with M. Overton and F. Rendl
TU Chemnitz

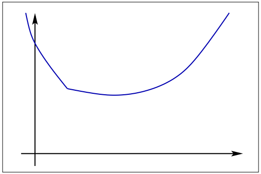
- The Bundle Method and the Aggregate
- SDP, Eigenvalue Optimisation, and the Spectral Bundle Method
- Second Order Approaches to Eigenvalue Optimisation
- Adaptation to the Spectral Bundle Method
- Numerical Examples
- Conclusions

Workshop "Semidefinite Programming: Theory and Applications"
Edinburgh, October 19, 2018

The Bundle Method for Nonsmooth Convex Optimization

$$\min \; f(y) \quad \text{s.t.} \quad y \in \mathbb{R}^m$$

with $f : \mathbb{R}^m \to \mathbb{R}$ convex (nonsmooth)



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f is specified by a **first order oracle**:

given $\bar{y} \in \mathbb{R}^m$ it returns

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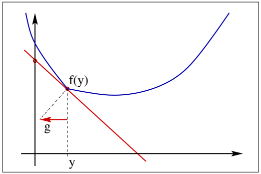
- $g(\bar{y}) \in \mathbb{R}^m$ some subgradient (not nec. unique)



satisfying $f(y) \geq f(\bar{y}) + \langle g(\bar{y}), y - \bar{y} \rangle \quad \forall y \in \mathbb{R}^m$ (subg. ineq.)

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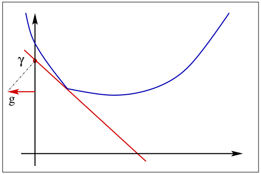

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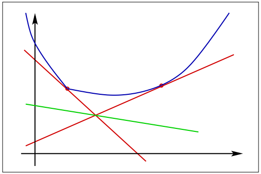

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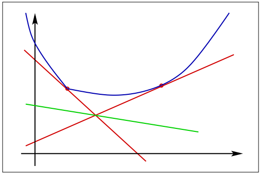

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Any closed proper convex function is the sup over its linear minorants,

$$f(y) = \sup_{(\gamma,g) \in \mathcal{W}} \gamma + \langle g, y \rangle, \qquad \text{choose compact } \widehat{\mathcal{W}} \subseteq \mathcal{W}.$$

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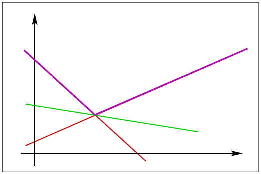

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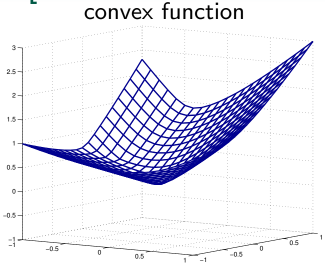
Maximizing over all $\omega \in \widehat{\mathcal{W}}$ gives a **cutting model** minorizing f,

$$f_{\widehat{\mathcal{W}}}(y) := \max_{\omega \in \widehat{\mathcal{W}}} f_\omega(y) \quad \leq f(y) \qquad \forall y \in \mathbb{R}^m$$

Proximal Bundle Method [Lemaréchal78,Kiwiel90]

Input: a convex function
given by a first order oracle



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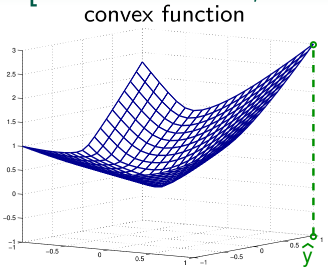

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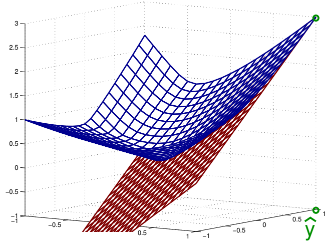
cutting plane model with $g \in \partial f(\hat{y})$



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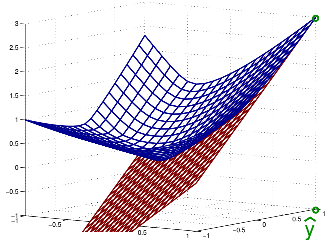

Input: a convex function
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1. Find a candidate by solving

$$\min_{y} \max_{\omega \in \widehat{\mathcal{W}}} f_\omega(y)$$

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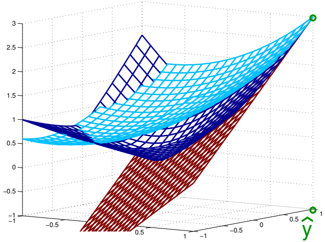
solve augmented model $\rightarrow \bar{y}$



Input: a convex function
given by a first order oracle

1. Find a candidate by solving the quadratic model

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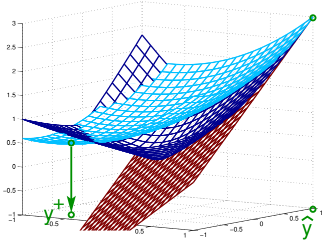

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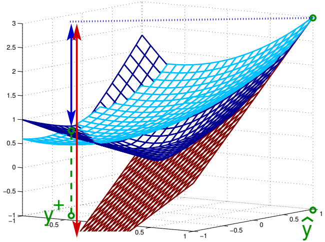

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3. Decide on
    - null step
    - descent step

Proximal Bundle Method [Lemaréchal78,Kiwiel90]

improve cutting model in $\bar{y}$

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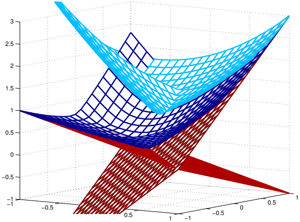

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3. Decide on
   - null step
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4. Update model to contain at least *aggregate* and new minorant and iterate

The Aggregate and Convergence

Given weight $\mu > 0$, the quadratic subproblem is a saddle point problem

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Determining the saddle point $(\bar{y}, \bar{\omega})$ over $\mathbb{R}^n \times \operatorname{conv} \widehat{\mathcal{W}}$ yields

- $\bar{\omega} = (\bar{\gamma}, \bar{g})$, the **aggregate** (the "best" minorant in $\operatorname{conv} \widehat{\mathcal{W}}$),
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Theorem (e.g. [BoGiLeSa2003])

Let $\hat{y}^k$ denote the center of iteration k, then $f(\hat{y}^k) \to \inf f$.
If, in addition, $\hat{y}^{k_0} = \hat{y}^k$ for $k \geq k_0$ (finitely many descent steps) then $\hat{y}^{k_0}$ minimizes f and $(f(\hat{y}^k) - f_{\bar{\omega}^k}(\bar{y}^k))_{k > k_0} \downarrow 0$.

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f bounded below $\Rightarrow \|\bar{g}^k\| \xrightarrow{K} 0$

The bundle framework offers a lot of flexibility and can be extended in many directions:

- add scaling/"second order" information via the proximal term
- allow constraints on y
- Lagrangian relaxation/decomposition or sums of convex functions
- generate good primal approximations in Lagrangian relaxation
- solve the dual to primal cutting plane approaches
- use specialized cutting models (quadratic subproblem solvable?)
- asynchronous parallel approaches

For me it offers the potential for

"A general tool like the simplex method for LP"

$\rightarrow$ ConicBundle, contains much but not yet all of this ...

Here: choose model and proximal term $+\frac{1}{2}\|y-\hat{y}\|_H^2$
for the maximum eigenvalue function/semidefinite prog.

LP $\leftrightarrow$ SDP

LP	SDP
$\max \; \langle c, x\rangle$ s.t. $Ax = b$, $x \geq 0$	$\max \; \langle C, X\rangle$ s.t. $\mathcal{A}X = b$, $X \succeq 0$
$x \in \mathbb{R}^n_+$ nonneg. orthant (polyhedral)	$X \in S^n_+$ pos. semidef. matrices (non-polyhedral)
$\langle c, x\rangle = \sum_i c_i x_i$	$\langle C, X\rangle = \sum_{i,j} C_{ij} X_{ij}$
$Ax = \begin{pmatrix} \langle a_1, x\rangle \\ \vdots \\ \langle a_m, x\rangle \end{pmatrix}$	$\mathcal{A}X = \begin{pmatrix} \langle A_1, X\rangle \\ \vdots \\ \langle A_m, X\rangle \end{pmatrix}$
$A^T y = \sum_i a_i y_i$	$\mathcal{A}^T y = \sum_i A_i y_i$
$\min \; \langle b, y\rangle$ s.t. $A^T y - z = c$, $z \geq 0$	$\min \; \langle b, y\rangle$ s.t. $\mathcal{A}^T y - Z = C$, $Z \succeq 0$

Example

$$\begin{aligned} \max \quad & \langle C, X \rangle \\ \text{s.t.} \quad & \langle I, X \rangle = 1 \\ & X \succeq 0 \end{aligned}$$

$$\begin{aligned} \min \quad & y \\ \text{s.t.} \quad & Z = yI - C \succeq 0 \end{aligned}$$

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set of primal optimal solutions:

$$\begin{aligned} & \operatorname{conv}\left\{vv^T : \left\langle I, vv^T\right\rangle = 1, v^T C v = \lambda_{\max}(C)\right\} \qquad [v = Pu] \\ = \; & \operatorname{conv}\left\{Puu^T P^T : \left\langle I, uu^T\right\rangle = 1\right\} \\ = \; & \left\{PUP^T : \langle I, U\rangle = 1, U \succeq 0\right\} \end{aligned}$$

columns of P form an orthonormal basis of the eigenspace of $\lambda_{\max}(C)$.

Spectral Bundle Method [H.,Rendl00]

For constant trace, the dual is an eigenvalue optimization problem

$$\begin{array}{rl} \max & \langle C, X\rangle \\ \text{s.t.} & \langle I, X\rangle = a \\ & \mathcal{A}X = b \\ & X \succeq 0, \end{array} \qquad \min_{y \in \mathbb{R}^m} \; a\lambda_{\max}(C - \mathcal{A}^T y) + \langle b, y\rangle$$

For bounded trace, the dual is

$$\begin{array}{rl} \max & \langle C, X\rangle \\ \text{s.t.} & \langle I, X\rangle \leq a \\ & \mathcal{A}X = b \\ & X \succeq 0, \end{array} \qquad \min_{y \in \mathbb{R}^m} \; \max\{0, a\lambda_{\max}(C - \mathcal{A}^T y)\} + \langle b, y\rangle$$

In the following we consider constant trace with $a = 1$,
and solve the eigenvalue problem by a specialized bundle approach.

The matrix $C - \sum_i A_i y_i$ inherits the structure of cost matrix and constraints [$\rightarrow$ $\lambda_{\max}$ by iterative methods like Lanczos]

A semidefinite model for $f(y) := \lambda_{\max}(C - \mathcal{A}^T y) + b^T y$

With $\mathcal{W} = \{W \succeq 0 : \operatorname{tr} W = 1\}$

$$f(y) = \max_{W \in \mathcal{W}} \langle W, C - \mathcal{A}^T y \rangle + b^T y$$

evaluate by computing $\lambda_{\max}(C - \mathcal{A}^T y)$, [Lanczos]
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$$\boxed{f_{\widehat{\mathcal{W}}_k}(y) = \max_{W \in \widehat{\mathcal{W}}_k} \langle W, C - \mathcal{A}^T y \rangle + b^T y} \qquad \le f(y) \quad \forall y \in \mathbb{R}^m$$

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We use

$$\boxed{\widehat{\mathcal{W}}_k = \left\{ P_k U P_k^T + \alpha \overline{X}_k : \operatorname{tr} U + \alpha = 1, U \succeq 0, \alpha \geq 0 \right\}} \qquad \subseteq \mathcal{W}$$

with parameters $P_k \in \mathbb{R}^{n \times r}$, $P_k^T P_k = I_r$, and an "aggregate" $\overline{X}_k \in \mathcal{W}$.

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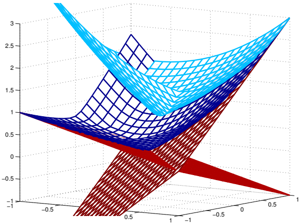
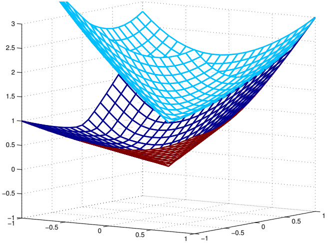
with parameters $P_k \in \mathbb{R}^{n \times r}$, $P_k^T P_k = I_r$, and an "aggregate" $\overline{X}_k \in \mathcal{W}$.
Convergence: $P = v$ and $\overline{X}$ or no $\overline{X}$ and big r with $\binom{r+1}{2} \le m$.

Spectral Bundle Model

cutting plane and augmented model



semidefinite model



Solving the augmented model $\min f_{\widehat{\mathcal{W}}}(y) + \frac{\mu}{2}\|y - \hat{y}\|^2$

$$\min_{y} \max_{W \in \widehat{\mathcal{W}}} \left\langle C - \mathcal{A}^T y, W \right\rangle + \langle b, y \rangle + \frac{\mu}{2}\|y - \hat{y}\|^2$$

$$= \max_{W \in \widehat{\mathcal{W}}} \min_{y} \langle C, W \rangle + \langle b - \mathcal{A}W, y \rangle + \frac{\mu}{2}\|y - \hat{y}\|^2$$

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Solve unconstrained quadratic inner optimization over y explicitly:

$$\boxed{y_+(W) = \hat{y} - \frac{1}{\mu}(b - \mathcal{A}W)}$$

[μ "step size/trust region control"]

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Substitute for y to obtain a quadratic semidefinite problem in W,

$$(\text{QSP}) \quad \begin{array}{ll} \min & \frac{1}{2\mu}\|b-\mathcal{A}W\|^2 - \left\langle W, C-\mathcal{A}^T\hat{y}\right\rangle - \langle b,\hat{y}\rangle \\ \text{s.t.} & W = PUP^T + \alpha\overline{X} \\ & \operatorname{tr} U + \alpha = 1 \\ & U \succeq 0, \alpha \geq 0. \end{array}$$

small if r is small ($U \in S^r_+$) $\rightarrow$ interior point system matrix $\binom{r+1}{2}+1$ [!]

$\rightarrow$ “best (eps)subgradient” $W_+ = PU_+P^T + \alpha_+\overline{X}$

$\rightarrow$ new candidate $y_+ = y_+(W_+)$.

Second Order Approaches

[Overton8*, OvertonWomersley95, Oustry200*]

Local quadratic convergence for correct multiplicity t in the optimum y^*,

$$C - \mathcal{A}^T y^* = [Q_1^* Q_2^*] \begin{bmatrix} \Lambda_1^* & 0 \\ 0 & \Lambda_2^* \end{bmatrix} [Q_1^* Q_2^*]^T$$

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1. Guess t_k, compute Q_1^k, Q_2^k and an interior subgradient U_k by

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2. Compute the Newton candidate by solving

$$\begin{array}{ll} \min & \frac{1}{2}\|y - \hat{y}_k\|_{H_k}^2 + \langle b, y\rangle + \delta \\ \text{s.t.} & \delta I = Q_1^T (C - \mathcal{A}^T y) Q_1 \end{array}$$

where

$$H_k = 2\mathcal{A}\left((Q_1 U_k Q_1^T) \otimes (Q_2[\lambda_1^k I - \Lambda_2^k]^{-1} Q_2^T)\right)\mathcal{A}^T \qquad \text{[regularity } \succ 0]$$

Adaptation of Step 2 for Spectral Bundle

Step 2 $\begin{array}{ll} \min & \frac{1}{2}\|y-\hat{y}\|_H^2 + \langle b, y\rangle + \delta \\ \text{s.t.} & \delta I = Q_1^T(C - \mathcal{A}^T y)Q_1 \end{array}$ is relaxed to

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Dualize, then $\boxed{y_+(W) = \hat{y} - H^{-1}(b - \mathcal{A}W)}$

$$\text{(QSP)} \quad \begin{array}{ll} \min & \frac{1}{2}\|b - \mathcal{A}W\|_{H^{-1}}^2 - \left\langle W, C - \mathcal{A}^T\hat{y}\right\rangle - \langle b, \hat{y}\rangle \\ \text{s.t.} & W = Q_1 U Q_1^T \\ & \operatorname{tr} U = 1 \\ & U \succeq 0. \end{array}$$

Scope of a second order bundle method

If QSP is solved by an interior point method with r columns, each iteration of QSP requires the factorization of a $\binom{r+1}{2}$ matrix.

For m constraints we can expect $r \approx \sqrt{m}$.
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Typically, a full interior point code requires several $O(n^3)$ and one $O(m^3)$ operation per iteration.

$\rightarrow$ Second order SB is unlikely to be attractive for $m \geq n$,
but might be relevant for small $m \leq n$ or if r is small.

$\rightarrow$ Emphasis on large n and rather small m.

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- **No scaling, bounded bundle (SB)**

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- **Diagonal Low-Rank (CB-diag):** Collect approximate subspace to large eigenvalues, use subgradient W_+ of (QSP) and the diagonal of the approximate Newton matrix $(+\rho I)$

Low Rank Structure

$$H = 2\mathcal{A}\left((Q_1 U Q_1^T) \otimes (Q_2[\lambda_1 I - \Lambda_2]^{-1} Q_2^T)\right)\mathcal{A}^T$$

decompose $U = Q_u \Lambda_u Q_u^T$, set $\bar{Q}_1 = Q_1 Q_u$ and rewrite H as

$$H = 2\mathcal{A}\left((\bar{Q}_1 \otimes Q_2)(\Lambda_u \otimes [\lambda_1 I - \Lambda_2]^{-1})(\bar{Q}_1 \otimes Q_2^T)\right)\mathcal{A}^T$$

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Truncate $[\lambda_1 I - \Lambda_2]_{1,\dots,h}$ and $Q_2 \to Q_h$,
compute a QR-decomposition of $\mathcal{A}(\bar{Q}_1 \otimes Q_h) \ \to \ Q_\mathcal{A} R$

$$H_h = 2Q_\mathcal{A} \underbrace{R(\Lambda_u \otimes [\lambda_1 I - \Lambda_2]^{-1}_{1,\dots,h})R^T}_{\to \ \tilde{Q}\Lambda_H \tilde{Q}^T, \ Q_H := Q_\mathcal{A}\tilde{Q}} Q_\mathcal{A}^T$$

truncate $\Lambda_H \to \hat{\Lambda}_H, \hat{Q}_H$

$$\to \quad \hat{H} = \rho I + 2\hat{Q}_H \hat{\Lambda}_H \hat{Q}_H^T$$

for some regularization parameter $\rho > 0$.

Implementation Details

Multiplicity Detection.

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Update of Q_2 for the Low Rank Representation?

Heuristic: dynamically enlarge $\overline{Q}$ in case of too many null steps

Numerical Experiments

Sparse SDP Random Generator: A_i nonzero submatrices of order p
small instances:

$n \in \{100, 300, 500\}$, $m \in \{100, 500, 1000\}$, $p \in \{3, 5, 7\}$

larger instances:

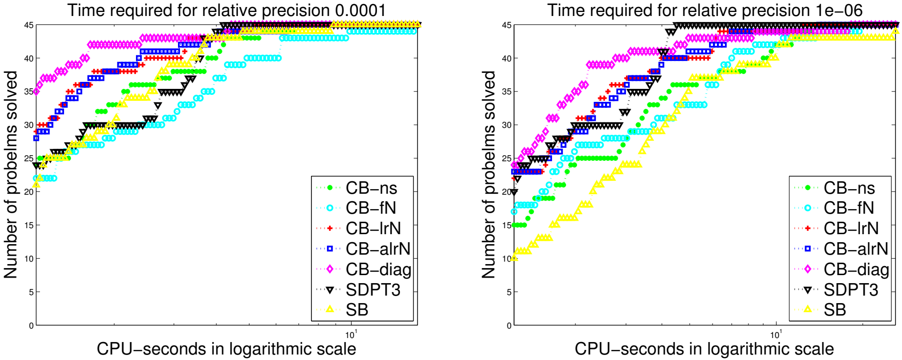
$n \in \{1, \ldots, 6\} \cdot 1000$, $m \in \{1, 3, 5\} \cdot 1000$, $p \in \{3, 4, 5\}$

Intel(R) Core(TM) i7 CPU 920 machines
8 MB cache, 12 GB RAM, openSUSE Linux 11.1 (x86_64)
in single processor mode

ConicBundle: start scaling at 10^{-2}
Termination: 10^{-8} or 10000 evaluations

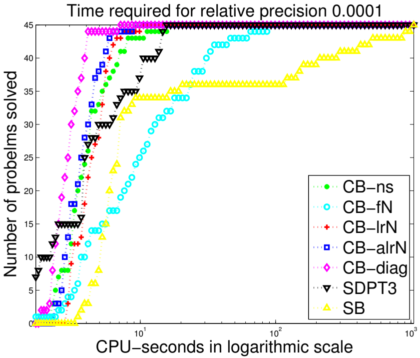
compare to SDPT3 4.0 beta [ToddTohTütüncü]

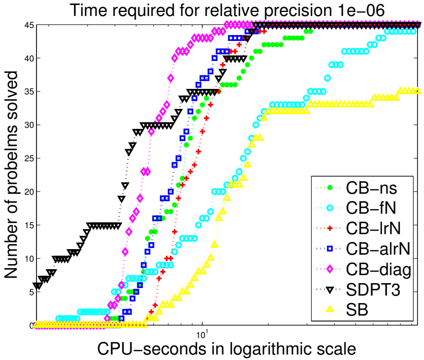
Small Instances: $n \in \{100, 300, 500\}$ and $m = 100$



Five instances per choice of n and constraint support order $\in \{3, 5, 7\}$

Small Instances: $n \in \{100, 300, 500\}$ and $m = 500$





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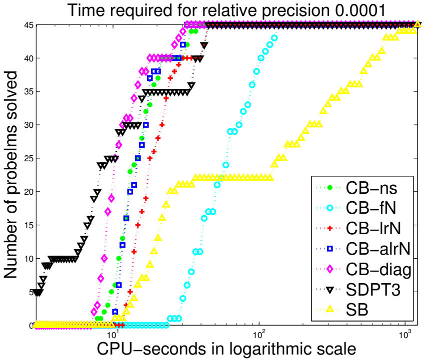

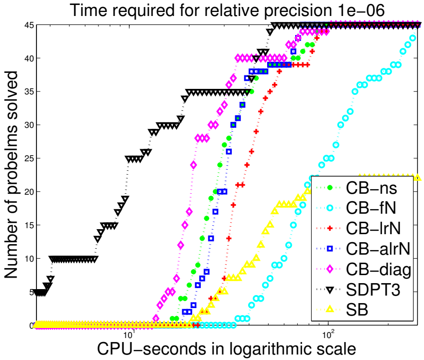

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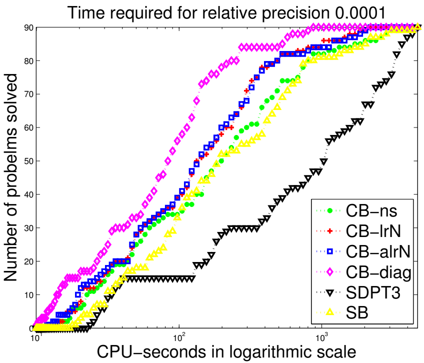
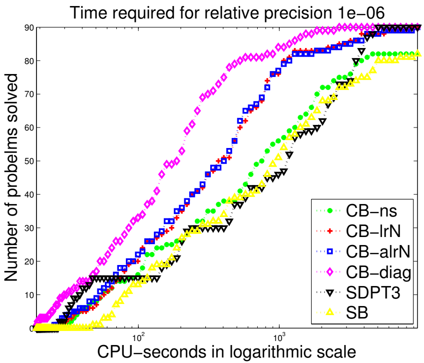
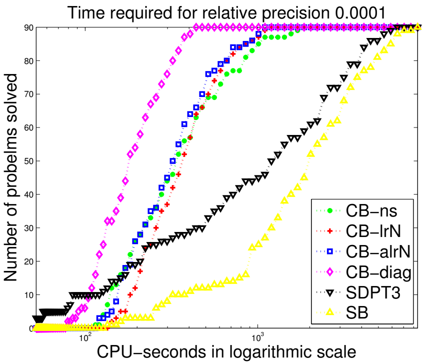
Larger Instances: $n \in \{1, \ldots, 6\} \cdot 1000$ and $m = 1000$

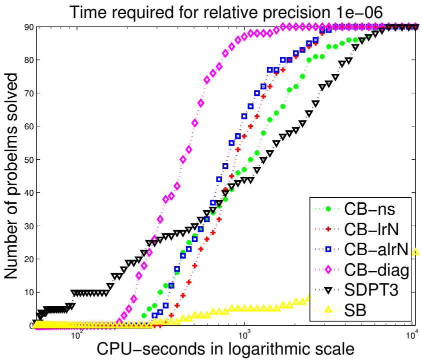




Five instances per choice of n and constraint support order $\in \{3, 4, 5\}$

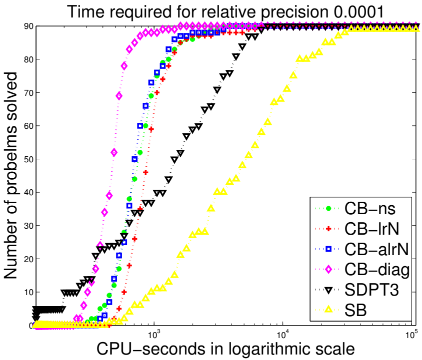
Larger Instances: $n \in \{1, \dots, 6\} \cdot 1000$ and $m = 3000$

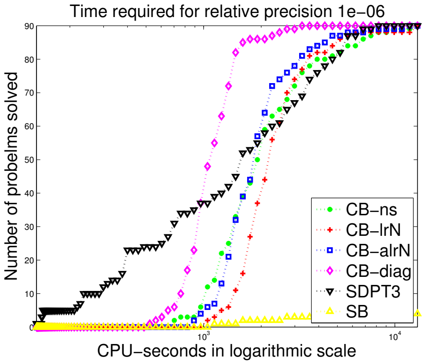




Five instances per choice of n and constraint support order $\in \{3, 4, 5\}$

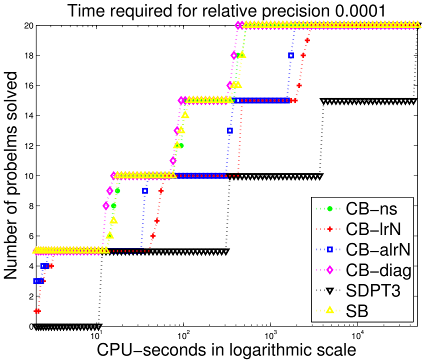
Larger Instances: $n \in \{1, \ldots, 6\} \cdot 1000$ and $m = 5000$

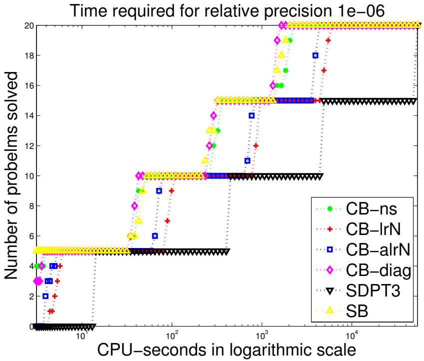




Five instances per choice of n and constraint support order $\in \{3, 4, 5\}$

Max-Cut 3D-Grids: n^3, $n \in \{10, 15, 20, 25\}$





Five instances with random ± 1 edge weights per choice of n

Number of Descent Steps, Small Instances

relative precision 10^{-6}, average and variance over 15 instances

n	m	CB-ns	CB-fN	CB-lrN	CB-alrN	CB-diag	SDPT3	SB
100	100	37 (6.11)	20 (3.44)	33 (6.86)	33 (6.09)	38 (21.3)	11 (0.573)	*43 (10.4)
300	100	43 (5.96)	22 (4.7)	38 (8.5)	39 (9.86)	37 (8.65)	13 (0.49)	53 (10.2)
500	100	58 (12.7)	27 (6.67)	50 (11.1)	51 (11.2)	52 (20)	14 (0.611)	69 (25.1)
100	500	42 (5.44)	27 (3.07)	42 (5.56)	42 (5.3)	50 (15.4)	11 (0.499)	*48 (3.35)
300	500	59 (11.1)	34 (5.04)	56 (10.2)	57 (11.3)	57 (11.6)	13 (0.806)	54 (6.3)
500	500	66 (11.5)	37 (5.23)	62 (12.2)	63 (12.4)	59 (15.9)	14 (0.596)	64 (15.6)
100	1000	51 (7)	32 (3.25)	50 (8.13)	49 (8.26)	60 (17.9)	10 (0.249)	*55 (2.46)
300	1000	59 (6.76)	36 (5.84)	59 (6.81)	59 (6.31)	60 (7.8)	12 (0.442)	*55 (3.26)
500	1000	67 (10.8)	42 (5.44)	67 (11.2)	67 (11.1)	67 (10.5)	13 (0.442)	*58 (3.64)

$*$ not all instances achieved the required precision

Number of Oracle Calls, Small Instances

relative precision 10^{-6}, average and variance over 15 instances

n	m	CB-ns	CB-fN	CB-lrN	CB-alrN	CB-diag	SDPT3	SB
100	100	75 (25.6)	44 (24.9)	49 (15.8)	52 (15.6)	54 (31.3)	11 (0.573)	255 (504)
300	100	155 (60.4)	75 (44.2)	104 (41.4)	110 (49.1)	86 (29.3)	13 (0.49)	279 (171)
500	100	314 (135)	95 (44.6)	195 (102)	199 (108)	163 (132)	14 (0.611)	464 (399)
100	500	83 (18.8)	68 (27.8)	69 (13.7)	68 (12.6)	76 (20.7)	11 (0.499)	*119453 ($1.03\cdot10^5$)
300	500	178 (110)	142 (132)	125 (46.3)	127 (54.4)	107 (32.3)	13 (0.806)	289 (207)
500	500	295 (211)	180 (129)	187 (99.9)	188 (99.8)	143 (75.5)	14 (0.596)	532 (462)
100	1000	117 (35.6)	90 (25.4)	96 (21)	97 (22.6)	113 (34)	10 (0.249)	*213306 ($3.65\cdot10^4$)
300	1000	151 (41.8)	110 (59.8)	123 (23.3)	124 (24.1)	118 (19.9)	12 (0.442)	*25553 ($3.58\cdot10^4$)
500	1000	238 (159)	152 (65.1)	177 (83.8)	178 (86.7)	148 (37)	13 (0.442)	*15803 ($3.12\cdot10^4$)

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$\rightarrow$ Scope of scaled CB: fast low precision results, cutting plane approaches, high precision results with large matrices and few constraints.

Thank you for your attention!