A symmetric extension of the NT direction

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based on joint work with C. Hergenroeder

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Why do iterative approaches for general purpose interior point methods pretty much fail so far?

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Can we overcome this?

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- Can we overcome this?
- I) LP

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- Can we overcome this?
- I) LP
- II) SDP and the NT direction

What do we need?

1. Avoid systematic cancellation errors in the transformations of the right hand side.

- 2. Generate linear systems with *bounded condition numbers*.
- 3. Preserve the *sparsity structure* of the constraints.
- 4. Generate *symmetric* systems.
- 5. Generate *positive definite* systems.

Analysis of the linear systems will be a bit technical

To get this implemented you just need to be stubborn and push it through

(I try to concentrate on the main points)

I) Linear Programs

minimize_{$$x \in IR^n$$} $c^T x$ subject to $Ax = b$ and $x \ge 0$,

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Interior point system:

$$Ax = b,$$

$$A^{T}y + s = c,$$

$$Xs = \mu e,$$

x > 0, s > 0 and $X := Diag(x_1, x_2, ..., x_n)$

Search direction

Let

$$p := b - Ax$$
, $q := c - A^T y - s$, and $r := \mu^+ e - Xs$.

"Standard System", (Std.S):

$$\begin{bmatrix} 0 & A & 0 \\ A^T & 0 & I \\ 0 & S & X \end{bmatrix} \begin{bmatrix} \Delta y \\ \Delta x \\ \Delta s \end{bmatrix} = \begin{bmatrix} p \\ q \\ r \end{bmatrix}.$$

Reduction to 2 by 2

Eliminating with any of the red diagonal matrices

$$\begin{bmatrix} 0 & A & 0 \\ A^T & 0 & I \\ 0 & S & X \end{bmatrix} \begin{bmatrix} \Delta y \\ \Delta x \\ \Delta s \end{bmatrix} = \begin{bmatrix} p \\ q \\ r \end{bmatrix}.$$

and diagonal scaling leads to

$$\begin{bmatrix} 0 & A \\ A^T & -SX^{-1} \end{bmatrix} \begin{bmatrix} \Delta y \\ u \end{bmatrix} = \begin{bmatrix} rhs1 \\ rhs2 \end{bmatrix},$$

with $u = \Delta x$ or $u = -XS^{-1}\Delta s$ and

$$\begin{bmatrix} rhs1\\ rhs2 \end{bmatrix} = \begin{bmatrix} p\\ q - X^{-1}r \end{bmatrix} \quad \text{or} \quad \begin{bmatrix} rhs1\\ rhs2 \end{bmatrix} = \begin{bmatrix} p - AS^{-1}r\\ q \end{bmatrix}$$

Systematic cancellation

The small entries of X or the small entries of S in

$$\begin{bmatrix} rhs1\\ rhs2 \end{bmatrix} = \begin{bmatrix} p\\ q - X^{-1}r \end{bmatrix} \quad \text{or} \quad \begin{bmatrix} rhs1\\ rhs2 \end{bmatrix} = \begin{bmatrix} p - AS^{-1}r\\ q \end{bmatrix}$$

lead to systematic cancellation error of entries in q or in p.

Pivoting:

Partition x and s into two parts, x_1 , x_2 and s_1 , s_2 such that

$$x_1 \ge s_1$$
 and $x_2 < s_2$.

 $(x_1 \text{ and } x_2 \text{ each have many components.})$

Stable reduction (Freund, J', 1993)

Defining

$$\tilde{q} := \begin{bmatrix} q_1 - X_1^{-1} r_1 \\ q_2 \end{bmatrix}$$
 and $\tilde{p} := p - A_2 S_2^{-1} r_2$,

the "Stable Reduction" (Stb.R) is given by

$$\begin{bmatrix} 0 & A \\ A^{T} & -SX^{-1} \end{bmatrix} \begin{bmatrix} \Delta y \\ u \end{bmatrix} = \begin{bmatrix} \tilde{p} \\ \tilde{q} \end{bmatrix}$$

where

$$u = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$$
, $u_1 := \Delta x_1$, and $u_2 := -X_2 S_2^{-1} \Delta s_2$.

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Normal equations

Eliminating again with the diagonal matrix SX^{-1} , any of the 2-by-2 systems leads to the same set of normal equations, **(Nrm.E)**

$$AXS^{-1}A^{T}\Delta y = p + AS^{-1}(Xq - r).$$

Small entries of X cancel components in q and small components of S cancel p.

Most commonly used with direct solvers.

Comparison

Condition numbers for small nondegenerate LPs (100×250) 100 random problems, *A* unitary, *x*, *s* nearly central:

μ	cond. (Std.S)	cond. (Stb.R)	cond. (Nrm.E)
1	210 (320/120)	1300 (2200/610)	10 (15/8)
10^{-4}	1.5e4 (3.5e5/2400)	3.8e8 (1.8e10/5.1e7)	6.1e5 (9.2e7/1.5e6)
10^{-8}	1.4e4 (1.1e6/3400)	2.7e12 (2.1e14/5.8e11)	5.0e5 (3.0e9/4.7e4)

(This does not reflect systematic cancellation – or symmetry)

Consequence: None of the systems seems suitable (and (Stb.R) seems worst)

Generally, no/few general purpose interior point methods using iterative solvers.

Extending instead of reducing?

Introduce a "dummy variable" $\Delta z := -X^{-1/2}\Delta x$.

Then,

$$\begin{bmatrix} 0 & A & 0 & 0 \\ A^{T} & 0 & I & 0 \\ 0 & I & 0 & X^{1/2} \\ 0 & 0 & X^{1/2} & -S \end{bmatrix} \begin{bmatrix} \Delta y \\ \Delta x \\ \Delta s \\ \Delta z \end{bmatrix} = \begin{bmatrix} p \\ q \\ 0 \\ \chi^{-1/2} r \end{bmatrix}$$

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(Still some cancellation with small entries of X)

Diagonal pivoting:

Pivoting as for (Stb.R) leads to a first symmetric extension



In case anybody likes to see:

 Δz has changed its meaning but $\Delta x, \Delta y, \Delta s$ remain the same: Solving the last two block rows for Δz we obtain

$$\Delta z = S^{-1} X^{1/2} \Delta s - \begin{bmatrix} S_1^{-1} X_1^{-1/2} r_1 \\ 0 \end{bmatrix}$$

and inserting this in the third and fourth block row yields

$$\Delta x + X^{1/2} \left(S^{-1} X^{1/2} \Delta s - \begin{bmatrix} S_1^{-1} X_1^{-1/2} r_1 \\ 0 \end{bmatrix} \right) = \begin{bmatrix} 0 \\ S_2^{-1} r_2 \end{bmatrix}.$$

Multiplying this from left with S yields $S\Delta x + X\Delta s = r$.

Symmetric diagonal scaling (last block row/column)

with
$$\text{Diag}(d)$$
 where $d_1 = x_1^{-1/2}$ and $d_2 = s_2^{-1/2}$ – leads to



the symmetric extension **(Sm.Ex)** (The meaning of Δz has changed again).

Reducing this again

Let

$$D_{x} := \begin{bmatrix} I & 0 \\ 0 & S_{2}^{-1/2} X_{2}^{1/2} \end{bmatrix}, \qquad D_{s} := \begin{bmatrix} X_{1}^{-1} S_{1} & 0 \\ 0 & I \end{bmatrix}.$$

The entries of D_x , D_s are nonnegative and at most 1.

Eliminating Δs with the second and third block row and Δx with the fourth and fifth block row leads to

(Rd.Ex)

$$\begin{bmatrix} 0 & AD_{x} \\ D_{x}A^{T} & D_{s} \end{bmatrix} \begin{bmatrix} \Delta y \\ \Delta z \end{bmatrix} = \begin{bmatrix} A \begin{bmatrix} 0 \\ S_{2}^{-1}r_{2} \end{bmatrix} - p \\ D_{x}q - \begin{bmatrix} X_{1}^{-1}r_{1} \\ 0 \end{bmatrix} \end{bmatrix}.$$

Given the (approximate) solution, the components Δx and Δs can be recovered in a stable fashion via

$$\Delta x = \begin{bmatrix} 0 \\ S_2^{-1} r_2 \end{bmatrix} - D_x \Delta z, \qquad \Delta s = q - A^T \Delta y.$$

This system will be denoted by "reduced extension" (Rd.Ex). Only cancellation error in q_2 ; recovered in back substitution!

Comparison

μ	cond. (Sm.Ex)	cond (Rd.Ex)	cond. opt. basis
1	43 (61/32)	18 (26/14)	320 (1.1e4/58)
1.0e-4	1100 (4.6e4/170)	350 (1.4e4/54)	280 (5700/52)
1.0e-8	820 (6.4e4/250)	250 (2.0e4/76)	250 (1.9e4/75)

Even far away from the central path, the condition of (Rd.Ex) and of the optimal basis are about the same when μ is small!

(Only about 30% of sQMR iterations compared to (Sm.Ex))

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Theorem

Assume that the LP has a unique (primal-dual) optimal solution and let $\bar{\kappa}$ be the 2-norm-condition number of the optimal basis. Assume further that the 2-norm of the optimal basis matrix and of its inverse are both at least 1.

For $\mu > 0$ let $x_{\mu}, y_{\mu}, s_{\mu}$ be any (not necessarily strictly) primal dual feasible solution with $x_{\mu}^{T} s_{\mu} \leq n\mu$. Let $\kappa(\mu)$ be the condition number of system **(Rd.Ex)** evaluated at x_{μ}, s_{μ} . Then, $\lim_{\mu \to 0} \kappa(\mu) = \bar{\kappa}$.

Moreover, (with $y_{\mu} := (AA^{T})^{-1}A(c - s_{\mu})$), the reduction

$$(\mathsf{Std}.\mathsf{S}) \longrightarrow (\mathsf{Rd}.\mathsf{Ex})$$

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is asymptotically stable for $\mu \rightarrow 0$.

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Proof:

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Proof: Straightforward. -

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II) SDP

Notation:

minimize_{X \in Sⁿ} $C \bullet X$ subject to A(X) = b and $X \succeq 0$,

where S^n is the space of symmetric $n \times n$ -matrices, $b \in IR^m$, $C \in S^n$, $C \bullet X := trace(CX)$, and

$$\mathcal{A}(X) = \begin{bmatrix} A^{(1)} \bullet X \\ \vdots \\ A^{(m)} \bullet X \end{bmatrix}, \qquad \mathcal{A}^*(y) = \sum_{i=1}^m y_i A^{(i)}.$$

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Central Path

Let \mathbf{S}_P denote the symmetrization operator introduced by Monteiro and Zhang,

$$\mathbf{S}_{P}(U) := \frac{1}{2}(PUP^{-1} + (PUP^{-1})^{T})$$

with some nonsingular matrix P.

The central path is defined by $X, S \succ 0, y \in I\!R^m$ with

$$\mathcal{A}(X) = b,$$

 $\mathcal{A}^*(y) + S = C,$
 $\mathbf{S}_P(XS) = \mu I.$

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(Std.S)

Let $X, S \succ 0, y \in IR^m$ be given, and set $p := b - A(X), \quad Q := C - A^*(y) - S, \text{ and } R := \mu^+ I - \mathbf{S}_P(XS)$ with some "target value" $\mu^+ (\leq X \bullet S/n)$. Newton's method yields

$$\begin{bmatrix} 0 & \mathcal{A} & 0 \\ \mathcal{A}^* & 0 & I \\ 0 & \mathbf{S}_P(..S) & \mathbf{S}_P(X.) \end{bmatrix} \begin{bmatrix} \Delta y \\ \Delta X \\ \Delta S \end{bmatrix} = \begin{bmatrix} p \\ Q \\ R \end{bmatrix}.$$

NT-direction

Let

$$W := S^{-1/2} (S^{1/2} X S^{1/2})^{1/2} S^{-1/2}$$

be the metric geometric mean of X and S^{-1} . Then,

$$WSW=X,\qquad S=W^{-1}XW^{-1},$$

$$W^{1/2}SW^{1/2}=W^{-1/2}XW^{-1/2}=:E\quad(=E(X,S)),$$
 and when $XS\approx\mu I,$ we have

$$E \approx \sqrt{\mu}I.$$

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Set $P := W^{-1/2}$.

"Scaling" operator $\mathcal{D}_P : \mathcal{S}^n \to \mathcal{S}^n$ and "Lyapunov operator" $\mathcal{L}_E : \mathcal{S}^n \to \mathcal{S}^n$ defined via

$$\mathcal{D}_{P}(\Delta X) := P \Delta X P$$
 and $\mathcal{L}_{E}(\Delta X) := rac{1}{2}(E \Delta X + \Delta X E).$

Then,

$$\mathbf{S}_{P}(\Delta XS) = \frac{1}{2} (P\Delta XSP^{-1} + (P\Delta XSP^{-1})^{T})$$
$$= \frac{1}{2} (P\Delta XP \underbrace{P^{-1}SP^{-1}}_{E} + (P\Delta XP \underbrace{P^{-1}SP^{-1}}_{E})^{T}) = \mathcal{L}_{E}\mathcal{D}_{P}(\Delta X)$$

and, likewise,

$$\mathbf{S}_P(X\Delta S) = \mathcal{L}_E \mathcal{D}_{P^{-1}}(\Delta S).$$

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Same system:

or

$$\begin{bmatrix} 0 & \mathcal{A} & 0 \\ \mathcal{A}^* & 0 & I \\ 0 & \mathcal{L}_E \mathcal{D}_P & \mathcal{L}_E \mathcal{D}_{P^{-1}} \end{bmatrix} \begin{bmatrix} \Delta y \\ \Delta X \\ \Delta S \end{bmatrix} = \begin{bmatrix} p \\ Q \\ R \end{bmatrix}.$$

$$\begin{bmatrix} 0 & \mathcal{A} & 0 \\ \mathcal{A}^* & 0 & I \\ 0 & \sqrt{\mu} \mathcal{D}_P & \sqrt{\mu} \mathcal{D}_{P^{-1}} \end{bmatrix} \begin{bmatrix} \Delta y \\ \Delta X \\ \Delta S \end{bmatrix} = \begin{bmatrix} p \\ Q \\ \sqrt{\mu} (\mathcal{L}_E)^{-1} R \end{bmatrix}.$$

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P and P^{-1} have same eigenbasis! (Unique to NT)

Unitary rescaling

Let $P = U\Lambda U^T$ be the eigenvalue decomposition of P, and $\mathcal{U} : S^n \to S^n$ be defined by $\mathcal{U}(Z) = UZU^T$ with adjoint $\mathcal{U}^*(Y) = \mathcal{U}^{-1}(Y) = U^T Y U$.

$$\begin{bmatrix} 0 & \mathcal{A}\mathcal{U} & 0 \\ \mathcal{U}^*\mathcal{A}^* & 0 & I \\ 0 & \sqrt{\mu}\mathcal{D}_{\Lambda} & \sqrt{\mu}\mathcal{D}_{\Lambda^{-1}} \end{bmatrix} \begin{bmatrix} \Delta y \\ \mathcal{U}^*\Delta X \\ \mathcal{U}^*\Delta S \end{bmatrix} = \begin{bmatrix} p \\ \mathcal{U}^*Q \\ \mathcal{U}^*\sqrt{\mu}(\mathcal{L}_E)^{-1}R \end{bmatrix},$$

Here, \mathcal{D}_{Λ} , $\mathcal{D}_{\Lambda^{-1}}$ are "true" diagonal scalings. $\mathcal{D}_{\Lambda}(M) = \Lambda M \Lambda = M \circ (\operatorname{diag}(\Lambda)e^{T} + e(\operatorname{diag}(\Lambda))^{T})$ (Hadamard product, $e = (1, 1, \dots, 1)^{T}$.) Iterative schemes only require multiplication with this matrix, not its representation.

In particular, \mathcal{AU} and $\mathcal{U}^*\mathcal{A}*$ are not formed explicitly.

Let $\widehat{\Delta X} := \mathcal{U}^* \Delta X$, $\widehat{\Delta S} := \mathcal{U}^* \Delta S$, and $\widehat{\Delta Z}$ be a dummy variable, set $\tilde{R} := \sqrt{\mu} (\mathcal{L}_E)^{-1} R$ then, (up to diagonal scaling) the symmetric extension is given by

Symmetric Extension

$$\begin{bmatrix} 0 & \mathcal{A}\mathcal{U} & 0 & 0 \\ \mathcal{U}^*\mathcal{A}^* & 0 & I & 0 \\ 0 & I & 0 & \sqrt[4]{\mu}\mathcal{D}_{\Lambda^{-1/2}} \\ 0 & 0 & \sqrt[4]{\mu}\mathcal{D}_{\Lambda^{-1/2}} & -\sqrt{\mu}\mathcal{D}_{\Lambda} \end{bmatrix} \begin{bmatrix} \Delta y \\ \widehat{\Delta X} \\ \widehat{\Delta S} \\ \widehat{\Delta Z} \end{bmatrix} = \begin{bmatrix} p \\ \mathcal{U}^*Q \\ \mathcal{U}^*R_2 \\ \mathcal{U}^*R_1 \end{bmatrix},$$

where

$$\sqrt{\mu}\mathcal{D}_{\Lambda}\mathcal{U}^*R_2 + \sqrt[4]{\mu}\mathcal{D}_{\Lambda^{-1/2}}\mathcal{U}^*R_1 = \mathcal{U}^*\tilde{R}$$

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Changing R_1 and R_2 s.t. to above constraint changes $\widehat{\Delta Z}$ but not $\Delta y, \widehat{\Delta X}, \widehat{\Delta S}$.

Chioce of ΔZ

► Minimizing ||R₁||²_F + ||R₂||²_F subject to above constraint can be solved explicitly (and cheaply),

$$(\mathcal{U}^* R_2)_{i,j} = (\mathcal{U}^* \tilde{R})_{i,j} \frac{\sqrt{\mu}\lambda_i\lambda_j}{\mu\lambda_i^2\lambda_j^2 + \sqrt{\mu}\lambda_i^{-1}\lambda_j^{-1}},$$
$$(\mathcal{U}^* R_1)_{i,j} = (\mathcal{U}^* \tilde{R})_{i,j} \frac{\sqrt[4]{\mu}\lambda_i^{-1/2}\lambda_j^{-1/2}}{\mu\lambda_i^2\lambda_j^2 + \sqrt{\mu}\lambda_i^{-1}\lambda_j^{-1}}.$$

– replacing the partition into x_1 and x_2 for LPs,

Chioce of ΔZ

► Minimizing ||R₁||²_F + ||R₂||²_F subject to above constraint can be solved explicitly (and cheaply),

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$$(\mathcal{U}^* R_1)_{i,j} = (\mathcal{U}^* \tilde{R})_{i,j} \frac{\sqrt[4]{\mu}\lambda_i^{-1/2}\lambda_j^{-1/2}}{\mu\lambda_i^2\lambda_j^2 + \sqrt{\mu}\lambda_i^{-1}\lambda_j^{-1}}.$$

– replacing the partition into x_1 and x_2 for LPs,

So, all the same as for LPs?

The Theorem ?

The partition $x_1 > s_1$ and $x_2 < s_2$ was crucial for the proof of the theorem for LPs.

Here, $\sqrt{\mu}\lambda_i^2 \rightarrow 0$ for some i, $\sqrt{\mu}\lambda_j^2 \rightarrow \infty$ for some j, and $\sqrt{\mu}\lambda_i\lambda_j \rightarrow const$ for some i, j.

 \implies Somewhat worse result, the right hand side may increase by a factor of $1/\sqrt[3]{\mu}.$

(Rd.Ex)

What we really aim for is the reduced extension which takes the form

$$\begin{bmatrix} 0 & L^{-1} \mathcal{A} \mathcal{U} \mathcal{D}_{\mathsf{X}} \\ \mathcal{D}_{\mathsf{X}} \mathcal{U}^* \mathcal{A}^* L^{-\mathsf{T}} & \mathcal{D}_{\mathsf{s}} \end{bmatrix} \begin{bmatrix} \widehat{\Delta y} \\ \widehat{\Delta Z} \end{bmatrix} = \begin{bmatrix} L^{-1} \mathcal{A} R_2 - L^{-1} p \\ \mathcal{D}_{\mathsf{X}} \mathcal{U}^* Q - \mathcal{D}_{\mathsf{M}} \mathcal{U}^* R_1 \end{bmatrix},$$

where we assume that a sparse Cholesky factor L of AA^* is available. (Not really crucial, but if available we like to use it.) Given $\widehat{\Delta y}$ get

$$\widehat{\Delta X} = \mathcal{U}^* R_2 - \mathcal{D}_x \widehat{\Delta Z}, \quad \widehat{\Delta S} = \mathcal{U}^* Q - \mathcal{U}^* \mathcal{A}^* L^{-T} \widehat{\Delta y}.$$

Details

Choose R_1 abd R_2 as to minimize the right hand side of this system subject to the constraint

$$\sqrt{\mu}\mathcal{D}_{\Lambda}\mathcal{U}^*R_2 + \sqrt[4]{\mu}\mathcal{D}_{\Lambda^{-1/2}}\mathcal{U}^*R_1 = \mathcal{U}^*\tilde{R}.$$

Use an adapted predictor corrector interior-point method. (Project the search direction onto the equations $A\Delta X = p$ and $A^*\Delta y + \Delta S = Q$.)

10% accuracy in the computation of the search direction (!)

 Not yet competitive with SDPNAL (but much faster than SEDUMI or SDPT3 for large problems)

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- Needs some form of preconditioning
- possibly recycling the previous predictor step in the initial approximation for QMR in the next predictor step.

- Not yet competitive with SDPNAL (but much faster than SEDUMI or SDPT3 for large problems)
- Needs some form of preconditioning
- possibly recycling the previous predictor step in the initial approximation for QMR in the next predictor step.
- A factor 10 faster than the "unbalanced symmetric extension".

Small dense SDP 50x50, 230 linear constraints

iteration	corr. qmr-steps	centrality	step length	$-\log_{10}\mu$
1	3	.88	.70	.58
2	10	2.1	.78	1.3
5	103	2.6	.74	3.1
6	121	1.5	.68	3.7
10	495	3.0	.66	6.1
11	485	3.0	.63	6.6
15	1000	3.2	.41	8.5
16	2000	2.6	.59	9.0

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The overall number of QMR Iterations was 15477.

Solution generated by the algorithm: $X^{alg}, y^{alg}, S^{alg}$ Exact optimal solution: $X^{opt}, y^{opt}, S^{opt}$.

$$\begin{aligned} \frac{\|\mathcal{A}(X^{alg}) - b\|_2}{\|b\|_2} &= 1, 4 \cdot 10^{-9}, \qquad \frac{X^{alg} \bullet S^{alg}}{\|X^{alg}\|_F \|S^{alg}\|_F} = 2.9 \cdot 10^{-8}, \\ \frac{\|\mathcal{A}^* y^{alg} + S^{alg} - C\|_F}{\|C\|_F} &= 5.0 \cdot 10^{-13}, \\ \frac{\|X^{alg} - X^{opt}\|_F}{\|X^{alg}\|_F} &= 0.008, \qquad \frac{\|S^{alg} - S^{opt}\|_F}{\|S^{alg}\|_F} = 1.1 \cdot 10^{-5}. \end{aligned}$$

Relative errors significantly larger (by a factor of more than 10^5) than the relative residuals.

 \implies optimal solution is not well conditioned.

Small dense LP 2500 variables, 230 linear constraints

iteration	corr. qmr-steps	centrality	step length	$-\log_{10}\mu$
1	3	.48	.54	.43
5	9	4,4	.27	2.4
10	110	3.3	.60	4.2
15	125	3.9	.42	5.3
20	287	2.0	.39	6.5
25	699	2.1	.34	7.9
28	1205	1.4	.69	9.0

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The overall number of QMR Iterations was 18700.

Larger SDP

X of dimension 2000×2000 , 100000 sparse linear constraints 38 Interior-Point-Iterations 4469 QMR iterations 5 hours (older desktop):

relative primal infeasibility: 5.2e-11, relative dual infeasibility: 1.6e-11, relative complementarity: 1.7e-08.

(Optimal solution and condition number unknown.)

Outlook

Further details on Optimization Online (tonight?)

Seems to work also for AHO (joint work with T. Davi)

Further details on Optimization Online (tonight?)-

Seems to work also for AHO (joint work with T. Davi)

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