Preconditioned saddle point problems in finite precision arithmetic

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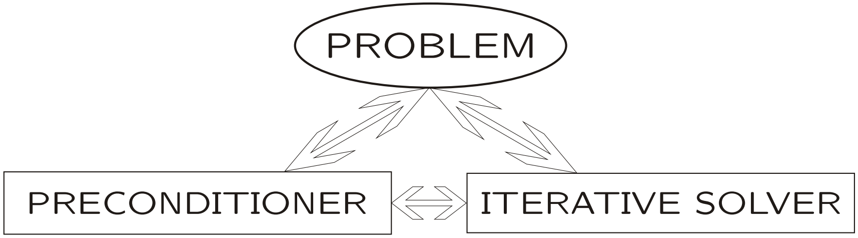
Saddle point problems

We consider a saddle point problem with the symmetric 2×2 block form

$$\begin{pmatrix} A & B \\ B^T & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix}.$$

- A is a square $n \times n$ nonsingular (symmetric positive definite) matrix,
- B is a rectangular $n \times m$ matrix of (full column) rank m.

Applications: mixed finite element approximations, weighted least squares, constrained optimization, computational fluid dynamics, electromagnetism etc. [Benzi, Golub and Liesen, 2005]. For the updated list of applications leading to saddle point problems contact [Benzi, 2009].

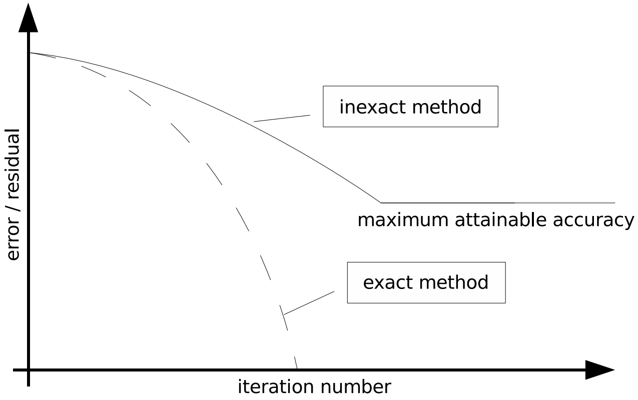

PROBLEM
PRECONDITIONER
ITERATIVE SOLVER

Iterative solution of saddle point problems

1. **segregated approach**: outer iteration for solving the reduced Schur complement or null-space projected system;
2. **coupled approach with block preconditioning**: iteration scheme for solving the preconditioned system;
3. **rounding errors in floating point arithmetic**: numerical stability of the solver

Numerous preconditioning techniques and schemes: block diagonal preconditioners, block triangular preconditioners, constraint preconditioning, Hermitian/skew-Hermitian preconditioning and other splittings, combination preconditioning
References: [Bramble and Pasciak, 1988], [Silvester and Wathen, Wathen and Silvester 1993, 1994], [Elman, Silvester and Wathen, 2002, 2005], [Kay, Loghin and Wathen, 2002], [Perugia, Simoncini, Arioli, 1999], [Keller, Gould and Wathen 2000], [Gould, Hribar and Nocedal, 2001], [Stoll, Wathen, 2008], ...

Delay of convergence and limit on the final accuracy



$\mathcal{A}$ symmetric indefinite, $\mathcal{P}$ positive definite

$$\mathcal{A} = \begin{pmatrix} A & B \\ B^T & 0 \end{pmatrix} \approx \mathcal{P} = \mathcal{R}^T \mathcal{R}$$

$$\left(\mathcal{R}^{-T} \mathcal{A} \mathcal{R}^{-1}\right) \mathcal{R} \begin{pmatrix} x \\ y \end{pmatrix} = \mathcal{R}^{-T} \begin{pmatrix} f \\ 0 \end{pmatrix}$$

$\mathcal{R}^{-T} \mathcal{A} \mathcal{R}^{-1}$ is symmetric indefinite!

Symmetric indefinite or nonsymmetric preconditioner

$\mathcal{P}$ symmetric indefinite or nonsymmetric

$$\mathcal{P}^{-1}\mathcal{A}\begin{pmatrix} x \\ y \end{pmatrix} = \mathcal{P}^{-1}\begin{pmatrix} f \\ 0 \end{pmatrix}$$

$$\left(\mathcal{A}\mathcal{P}^{-1}\right)\mathcal{P}\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix}$$

$\mathcal{P}^{-1}\mathcal{A}$ and $\mathcal{A}\mathcal{P}^{-1}$ are nonsymmetric!

Schur complement approach with indefinite preconditioner

$$\begin{pmatrix} A & B \\ B^T & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix}, \quad \mathcal{P} = \begin{pmatrix} A & B \\ B^T & B^T A^{-1} B - I \end{pmatrix}$$

$$\mathcal{A}\mathcal{P}^{-1} = \begin{pmatrix} I & 0 \\ (I - S) B^T A^{-1} & S \end{pmatrix}$$

$S = B^T A^{-1} B$, $\mathcal{A}\mathcal{P}^{-1}$ **nonsymmetric** but **diagonalizable** and it has a 'nice' spectrum!

$$\sigma(\mathcal{A}\mathcal{P}^{-1}) \subset \{1\} \cup \sigma(B^T A^{-1} B^T)$$

[Durazzi, Ruggiero 2003], [Fortin, El-Maliki, 2009?]

Krylov method with the preconditioner: basic properties

$$\begin{pmatrix} x_0 \\ y_0 \end{pmatrix}, r_0 = \begin{pmatrix} 0 \\ s_0 \end{pmatrix}, e_{k+1} = \begin{pmatrix} x - x_{k+1} \\ y - y_{k+1} \end{pmatrix}$$

$$r_{k+1} = \begin{pmatrix} f \\ 0 \end{pmatrix} - \begin{pmatrix} A & B \\ B^T & 0 \end{pmatrix} \begin{pmatrix} x_{k+1} \\ y_{k+1} \end{pmatrix}$$

$$r_0 = \begin{pmatrix} 0 \\ s_0 \end{pmatrix} \Rightarrow r_{k+1} = \begin{pmatrix} 0 \\ s_{k+1} \end{pmatrix}$$

$$\Rightarrow Ax_{k+1} + By_{k+1} = f$$

Preconditioned CG method: saddle point problem and indefinite preconditioner

$$r_{k+1}^T \mathcal{P}^{-1} r_j = 0,\ j = 0, \dots, k$$

y_{k+1} is an iterate from CG applied to the Schur complement system

$$B^T A^{-1} B y = B^T A^{-1} f!$$

satisfying

$$\|y - y_{k+1}\|_{B^T A^{-1} B} =$$
$$\min_{u \in x_0 + K_{k+1}(B^T A^{-1} B, B^T A^{-1} f)} \|y - u\|_{B^T A^{-1} B}$$

Preconditioned CG algorithm

$$\begin{pmatrix} x_0 \\ y_0 \end{pmatrix},\ r_0 = b - \mathcal{A}\begin{pmatrix} x_0 \\ y_0 \end{pmatrix} = \begin{pmatrix} 0 \\ s_0 \end{pmatrix}$$

$$\begin{pmatrix} p_0^{(x)} \\ p_0^{(y)} \end{pmatrix} = \mathcal{P}^{-1} r_0 = \mathcal{P}^{-1}\begin{pmatrix} 0 \\ s_0 \end{pmatrix}$$

$k = 0, 1, \ldots$

$$\alpha_k = \left(\begin{pmatrix} 0 \\ s_k \end{pmatrix}, \mathcal{P}^{-1}\begin{pmatrix} 0 \\ s_k \end{pmatrix}\right) / \left(\mathcal{A}\begin{pmatrix} p_k^{(x)} \\ p_k^{(y)} \end{pmatrix}, \begin{pmatrix} p_k^{(x)} \\ p_k^{(y)} \end{pmatrix}\right) \qquad \alpha_k = \frac{(r_k, z_k)}{(\mathcal{A}p_k, p_k)}$$

$$\begin{pmatrix} x_{k+1} \\ y_{k+1} \end{pmatrix} = \begin{pmatrix} x_k \\ y_k \end{pmatrix} + \alpha_k \begin{pmatrix} p_k^{(x)} \\ p_k^{(y)} \end{pmatrix}$$

$$r_{k+1} = r_k - \alpha_k \mathcal{A}\begin{pmatrix} p_k^{(x)} \\ p_k^{(y)} \end{pmatrix} = \begin{pmatrix} 0 \\ s_{k+1} \end{pmatrix} \qquad z_{k+1} = \mathcal{P}^{-1} r_{k+1}$$

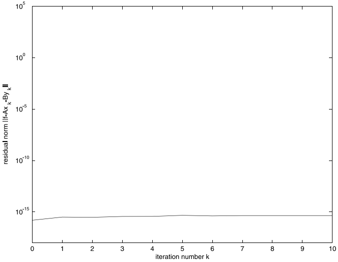
$$\beta_k = \left(\begin{pmatrix} 0 \\ s_{k+1} \end{pmatrix}, \mathcal{P}^{-1}\begin{pmatrix} 0 \\ s_{k+1} \end{pmatrix}\right) / \left(\begin{pmatrix} 0 \\ s_k \end{pmatrix}, \mathcal{P}^{-1}\begin{pmatrix} 0 \\ s_k \end{pmatrix}\right) \qquad \beta_k = \frac{(r_{k+1}, z_{k+1})}{(r_k, z_k)}$$

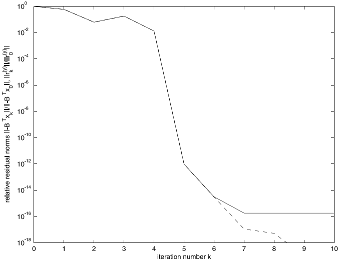
$$\begin{pmatrix} p_{k+1}^{(x)} \\ p_{k+1}^{(y)} \end{pmatrix} = \mathcal{P}^{-1}\begin{pmatrix} 0 \\ s_{k+1} \end{pmatrix} + \beta_k \begin{pmatrix} p_k^{(x)} \\ p_k^{(y)} \end{pmatrix} = \begin{pmatrix} -A^{-1} B p_{k+1}^{(y)} \\ p_{k+1}^{(y)} \end{pmatrix} \qquad p_{k+1} = z_{k+1} + \beta_k p_k$$

Numerical experiments: a small model example

$$A = \mathrm{tridiag}(1,4,1) \in \mathbb{R}^{25\times 25},\; B = \mathrm{rand}(25,5),\; f = \mathrm{rand}(25,1),$$
$$\kappa(A) = \|A\| \cdot \|A^{-1}\| = 5.9854 \cdot 0.4963 \approx 2.9710,$$
$$\kappa(B) = \|B\| \cdot \|B^{\dagger}\| = 5.9990 \cdot 0.4998 \approx 2.9983.$$

Generic update: $x_{k+1} = x_k + \alpha_k p_k^{(x)}$ with $p_k^{(x)} = -A^{-1} B p_k^{(y)}$





Saddle point problem and indefinite constraint preconditioner

$$\begin{pmatrix} A & B \\ B^T & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix}, \quad \mathcal{P} = \begin{pmatrix} I & B \\ B^T & 0 \end{pmatrix}$$

$$\mathcal{A}\mathcal{P}^{-1} = \begin{pmatrix} A(I-\Pi)+\Pi & (A-I)B(B^TB)^{-1} \\ 0 & I \end{pmatrix}$$

$\Pi = B(B^TB)^{-1}B^T$ - orth. projector onto $span(B)$

[Lukšan, Vlček, 1998], [Gould, Keller, Wathen 2000]
[Perugia, Simoncini, Arioli, 1999], [R, Simoncini, 2002]

Indefinite constraint preconditioner: spectral properties

$\mathcal{A}\mathcal{P}^{-1}$ **nonsymmetric** and **non-diagonalizable**!
but it has a 'nice' spectrum:

$$\begin{aligned}\sigma(\mathcal{A}\mathcal{P}^{-1}) &\subset \{1\} \cup \sigma(A(I-\Pi)+\Pi)\\ &\subset \{1\} \cup \sigma((I-\Pi)A(I-\Pi)) - \{0\}\end{aligned}$$

and only 2 by 2 Jordan blocks!

[Lukšan, Vlček 1998], [Gould, Wathen, Keller, 1999], [Perugia, Simoncini 1999]

Krylov method with the constraint preconditioner: basic properties

$$\begin{pmatrix} x_0 \\ y_0 \end{pmatrix}, r_0 = \begin{pmatrix} s_0 \\ 0 \end{pmatrix}, e_{k+1} = \begin{pmatrix} x - x_{k+1} \\ y - y_{k+1} \end{pmatrix}$$

$$r_{k+1} = \begin{pmatrix} f \\ 0 \end{pmatrix} - \begin{pmatrix} A & B \\ B^T & 0 \end{pmatrix} \begin{pmatrix} x_{k+1} \\ y_{k+1} \end{pmatrix}$$

$$r_0 = \begin{pmatrix} s_0 \\ 0 \end{pmatrix} \Rightarrow r_{k+1} = \begin{pmatrix} s_{k+1} \\ 0 \end{pmatrix}$$

$$\Rightarrow B^T(x - x_{k+1}) = 0$$

$$\Rightarrow x_{k+1} \in Null(B^T)!$$

Preconditioned CG algorithm

$$\begin{pmatrix} x_0 \\ y_0 \end{pmatrix},\ r_0 = b - \mathcal{A}\begin{pmatrix} x_0 \\ y_0 \end{pmatrix} = \begin{pmatrix} s_0 \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} p_0^{(x)} \\ p_0^{(y)} \end{pmatrix} = \mathcal{P}^{-1} r_0 = \mathcal{P}^{-1}\begin{pmatrix} s_0 \\ 0 \end{pmatrix}$$

$k = 0, 1, \ldots$

$$\alpha_k = \left(\begin{pmatrix} s_k \\ 0 \end{pmatrix}, \mathcal{P}^{-1}\begin{pmatrix} s_k \\ 0 \end{pmatrix}\right) / \left(\mathcal{A}\begin{pmatrix} p_k^{(x)} \\ p_k^{(y)} \end{pmatrix}, \begin{pmatrix} p_k^{(x)} \\ p_k^{(y)} \end{pmatrix}\right) \qquad \alpha_k = (r_k, z_k)/(\mathcal{A}p_k, p_k)$$

$$\begin{pmatrix} x_{k+1} \\ y_{k+1} \end{pmatrix} = \begin{pmatrix} x_k \\ y_k \end{pmatrix} + \alpha_k \begin{pmatrix} p_k^{(x)} \\ p_k^{(y)} \end{pmatrix}$$

$$r_{k+1} = r_k - \alpha_k \mathcal{A}\begin{pmatrix} p_k^{(x)} \\ p_k^{(y)} \end{pmatrix} = \begin{pmatrix} s_{k+1} \\ 0 \end{pmatrix} \qquad z_{k+1} = \mathcal{P}^{-1} r_{k+1}$$

$$\beta_k = \left(\begin{pmatrix} s_{k+1} \\ 0 \end{pmatrix}, \mathcal{P}^{-1}\begin{pmatrix} s_{k+1} \\ 0 \end{pmatrix}\right) / \left(\begin{pmatrix} s_k \\ 0 \end{pmatrix}, \mathcal{P}^{-1}\begin{pmatrix} s_k \\ 0 \end{pmatrix}\right) \qquad \beta_k = (r_{k+1}, z_{k+1})/(r_k, z_k)$$

$$\begin{pmatrix} p_{k+1}^{(x)} \\ p_{k+1}^{(y)} \end{pmatrix} = \mathcal{P}^{-1}\begin{pmatrix} s_{k+1} \\ 0 \end{pmatrix} + \beta_k \begin{pmatrix} p_k^{(x)} \\ p_k^{(y)} \end{pmatrix} \qquad p_{k+1} = z_{k+1} + \beta_k p_k$$

Preconditioned CG method: error norm

$$r_{k+1}^T \mathcal{P}^{-1} r_j = 0, \; j = 0, \ldots, k$$

x_{k+1} is an iterate from CG applied to

$$(I - \Pi) A (I - \Pi) x = (I - \Pi) f!$$

satisfying

$$\|x - x_{k+1}\|_A = \min_{u \in x_0 + span\{(I - \Pi) s_j\}} \|x - u\|_A$$

[Lukšan, Vlček 1998], [Gould, Wathen, Keller, 1999]

Preconditioned CG method: residual norm

$$\|x_{k+1} - x\| \to 0$$

but in general

$$y_{k+1} \not\to y$$

which is reflected in

$$\|r_{k+1}\| = \left\| \begin{pmatrix} s_{k+1} \\ 0 \end{pmatrix} \right\| \not\to 0!$$

but under appropriate scaling yes!

Preconditioned CG method: residual norm

$$x_{k+1} \to x$$

$$x - x_{k+1} = \phi_{k+1}((I - \Pi)A(I - \Pi))(x - x_0)$$

$$s_{k+1} = \phi_{k+1}(A(I - \Pi) + \Pi)s_0$$

$$\sigma((I - \Pi)A(I - \Pi)) \sim \sigma(A(I - \Pi) + \Pi)?$$

$$\{1\} \in \sigma((I - \Pi)\alpha A(I - \Pi)) - \{0\}$$
$$\Rightarrow \|r_{k+1}\| = \left\| \begin{pmatrix} s_{k+1} \\ 0 \end{pmatrix} \right\| \to 0!$$

How to avoid misconvergence?

- Scaling by a constant $\alpha > 0$ such that

$$\{1\} \in conv(\sigma((I-\Pi)\alpha A(I-\Pi)) - \{0\})$$

$$\begin{pmatrix} A & B \\ B^T & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix} \quad \Longleftrightarrow \quad \begin{pmatrix} \alpha A & B \\ B^T & 0 \end{pmatrix} \begin{pmatrix} x \\ \alpha y \end{pmatrix} = \begin{pmatrix} \alpha f \\ 0 \end{pmatrix}$$

$$v : \quad \|(I-\Pi)v\| \neq 0, \quad \alpha = \frac{1}{((I-\Pi)v, A(I-\Pi)v)}!$$

- Scaling by a diagonal $A \to (diag(A))^{-1/2} A (diag(A))^{-1/2}$ often gives what we want!
- Different direction vector $p_k^{(y)}$ so that $\|r_{k+1}\| = \|s_{k+1}\|$ is locally minimized!

$$y_{k+1} = y_k + (B^T B)^{-1} B^T s_k$$

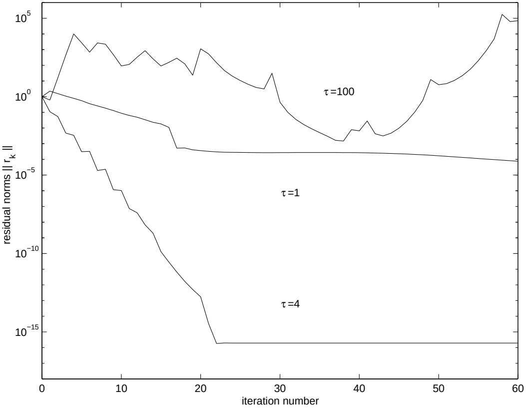
[Braess, Deuflhard,Lipikov 1999], [Hribar, Gould, Nocedal, 1999], [Jiránek, R, 2008]

Numerical experiments: a small model example

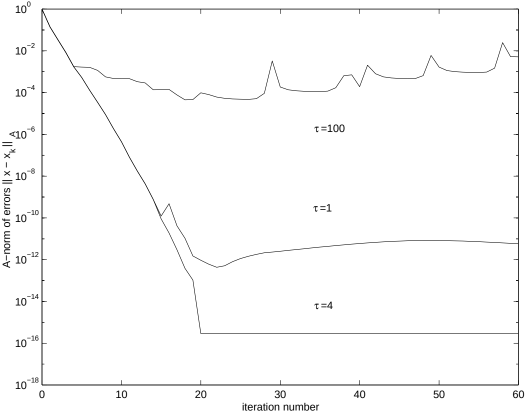
$$A = \mathrm{tridiag}(1,4,1) \in \mathsf{R}^{25,25},\ B = \mathrm{rand}(25,5) \in \mathsf{R}^{25,5}$$
$$f = \mathrm{rand}(25,1) \in \mathsf{R}^{25}$$

$$\sigma(A) \subset [2.0146, 5.9854]$$

$\alpha = 1/\tau$	$\sigma(\begin{pmatrix} \alpha A & B \\ B^T & 0 \end{pmatrix} \begin{pmatrix} I & B \\ B^T & 0 \end{pmatrix}^{-1})$
$1/100$	$[0.0207, 0.0586] \cup \{1\}$
$1/10$	$[0.2067, 0.5856] \cup \{1\}$
$\mathbf{1/4}$	$[\mathbf{0.5170}, \mathbf{1.4641}]$
1	$\{1\} \cup [2.0678, 5.8563]$
4	$\{1\} \cup [8.2712, 23.4252]$



10^{5}
10^{0}
10^{-5}
10^{-10}
10^{-15}
residual norms || r_k ||
0
10
20
30
40
50
60
iteration number
τ =100
τ =1
τ =4



A−norm of errors || x − x_k ||_A
iteration number
τ =100
τ =1
τ =4
10^0
10^−2
10^−4
10^−6
10^−8
10^−10
10^−12
10^−14
10^−16
10^−18
0
10
20
30
40
50
60

Error norm of the computed approximate solution

Finite precision arithmetic:

$$\begin{pmatrix} \bar{x}_{k+1} \\ \bar{y}_{k+1} \end{pmatrix}, \quad \bar{r}_{k+1} = \begin{pmatrix} \bar{s}^{(1)}_{k+1} \\ \bar{s}^{(2)}_{k+1} \end{pmatrix} \to 0$$

$$\|x - \bar{x}_{k+1}\|_A^2 = (\Pi A(x - \bar{x}_{k+1}), \Pi(x - \bar{x}_{k+1})) + ((I - \Pi)A(x - \bar{x}_{k+1}), (I - \Pi)(x - \bar{x}_{k+1}))$$

$$\|x - \bar{x}_{k+1}\|_A \le \gamma_1 \|\Pi(x - \bar{x}_{k+1})\| + \gamma_2 \|(I - \Pi)A(I - \Pi)(x - \bar{x}_{k+1})\|$$

Exact arithmetic:

$$\|\Pi(x - x_{k+1})\| = 0$$

$$\|(I - \Pi)A(I - \Pi)(x - x_{k+1})\| \to 0$$

Error norm of the computed approximate solution

departure from the null-space of B^T + projection of the residual onto it

$$\|x - \bar{x}_{k+1}\|_A \leq \gamma_3 \|B^T(x - \bar{x}_{k+1})\| + \gamma_2 \|(I - \Pi)(f - A\bar{x}_{k+1} - B\bar{y}_{k+1})\|$$

can be monitored by easily computable quantities:

$$B^T(x - \bar{x}_{k+1}) \sim \bar{s}_{k+1}^{(2)}$$

$$(I - \Pi)(f - A\bar{x}_{k+1} - B\bar{y}_{k+1}) \sim (I - \Pi)\bar{s}_{k+1}^{(1)}$$

Residuals: maximum attainable accuracy

$$\|(f - A\bar{x}_{k+1} - B\bar{y}_{k+1}) - \bar{s}^{(1)}_{k+1}\|, \ \|B^T(x - \bar{x}_{k+1}) - \bar{s}^{(2)}_{k+1}\| \leq$$

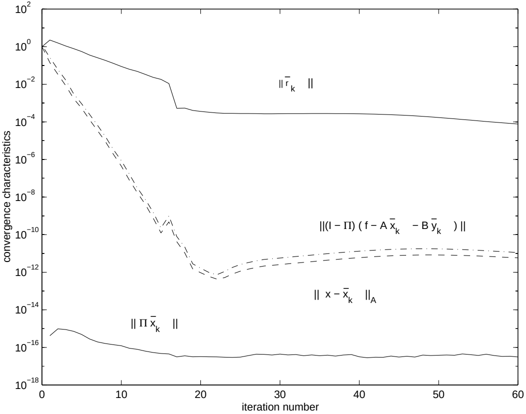
$$\leq \| \begin{pmatrix} f \\ 0 \end{pmatrix} - \begin{pmatrix} A & B \\ B^T & 0 \end{pmatrix} \begin{pmatrix} \bar{x}_{k+1} \\ \bar{y}_{k+1} \end{pmatrix} - \begin{pmatrix} \bar{s}^{(1)}_{k+1} \\ \bar{s}^{(2)}_{k+1} \end{pmatrix} \|$$

$$\leq c_1 \varepsilon \kappa(\mathcal{A}) \max_{j=0,\ldots,k+1} \|\bar{r}_j\|$$

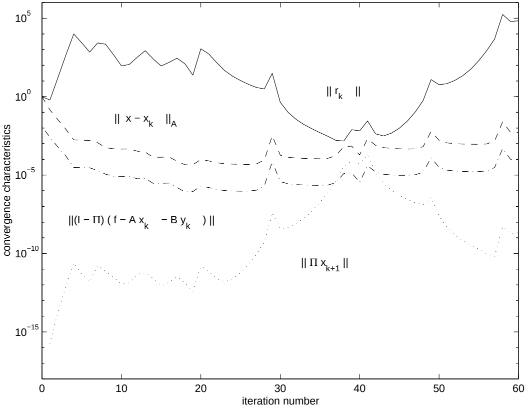
[Greenbaum 1994,1997], [Sleijpen, et al. 1994]

good scaling: $\|\bar{r}_j\| \to 0$ nearly monotonically

$\|\bar{r}_0\| \sim \max_{j=0,\ldots,k+1} \|\bar{r}_j\|$



convergence characteristics
iteration number
|| r̄_k ||
||(I − Π) (f − A x̄_k − B ȳ_k) ||
|| x − x̄_k ||_A
|| Π x̄_k ||



10^5
10^0
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10^−10
10^−15
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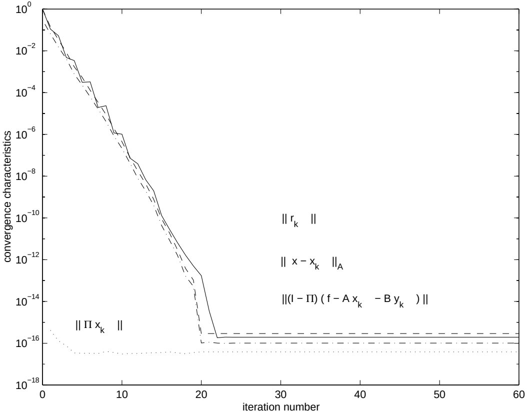
60
iteration number
convergence characteristics
|| r_k ||
|| x − x_k ||_A
||(I − Π) (f − A x_k − B y_k) ||
|| Π x_{k+1} ||


10^0
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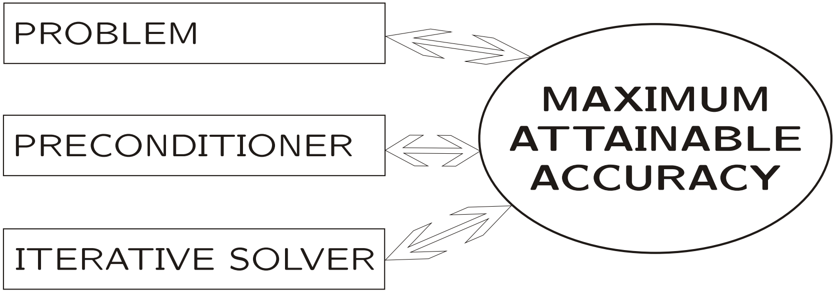
60
iteration number
|| r_k ||
|| x − x_k ||_A
||(I − Π) (f − A x_k − B y_k) ||
|| Π x_k ||


PROBLEM
PRECONDITIONER
ITERATIVE SOLVER
MAXIMUM ATTAINABLE ACCURACY

Conclusions: coupled approach with indefinite preconditioner

- Short-term recurrence methods are applicable for saddle point problems with indefinite preconditioning at a cost comparable to that of symmetric solvers. There is a tight connection between the simplified Bi-CG algorithm and the classical CG.
- The convergence of CG applied to saddle point problem with indefinite preconditioner for all right-hand side vectors is not guaranteed. For a particular set of right-hand sides the convergence can be achieved by the appropriate scaling of the saddle point problem.
- Since the maximum attainable accuracy depends heavily on the size of computed residuals, a good scaling of the problems leads to approximate solutions satisfying both two block equations to the working accuracy.

Thank you for your attention.

http://www.cs.cas.cz/∼miro

M. Rozložník and V. Simoncini, Krylov subspace methods for saddle point problems with indefinite preconditioning,*SIAM J. Matrix Anal. Appl., 24 (2002), pp. 368–391.*

P. Jiránek and M. Rozložník. Limiting accuracy of segregated solution methods for nonsymmetric saddle point problems. *J. Comput. Appl. Math.* 215 (2008), pp. 28-37.

P. Jiránek and M. Rozložník. Maximum attainable accuracy of inexact saddle point solvers. *SIAM J. Matrix Anal. Appl.*, 29(4):1297–1321, 2008.