SADDLE POINT SOLVERS AND THEIR NUMERICAL BEHAVIOR

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joint results with
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Workshop on Solution methods for Saddle Point Problems,
Hong Kong Baptist University, Hong Kong , October 31, 2007

OUTLINE

1. SYMMETRIC INDEFINITE SYSTEM + POSITIVE DEFINITE PRECONDITIONER: CG OR MINRES (OR SYMMLQ) METHOD

2. SYMMETRIC INDEFINITE SYSTEM + INDEFINITE PRECONDITIONER:
   SIMPLIFIED BI-CG OR QMR METHOD $\Longleftrightarrow$ PRECONDITIONED CG METHOD

3. **INDEFINITE SADDLE POINT PROBLEMS + INDEFINITE (CONSTRAINT OR PROJECTION) PRECONDITIONERS: PRECONDITIONED CG METHOD**

SYMMETRIC INDEFINITE SYSTEM, SYMMETRIC POSITIVE DEFINITE PRECONDITIONER

$$Ax = b$$

A symmetric indefinite, M positive definite

$$M^{-1/2}AM^{-T/2}y = M^{-1/2}b, \qquad x = M^{-T/2}y$$

$\tilde{A}\tilde{x} = \tilde{b}$, $\quad \tilde{A}$ symmetric (indefinite)!

ITERATIVE SOLUTION OF PRECONDITIONED (SYMMETRIC INDEFINITE) SYSTEM

PRECONDITIONED MINRES (MR), SYMMLQ (ME) - VARIOUS IMPLEMENTATIONS

CG APPLIED TO SYMMETRIC BUT INDEFINITE SYSTEM:

CG iterate exists at least at every second step (tridiagonal form T_n is nonsingular at least at every second step)

Paige, Saunders, 1975

peak/plateau behavior:
CG converges fast $\rightarrow$ MINRES is not much better than CG
CG norm increases (peak) $\rightarrow$ MINRES stagnates (plateau)

Greenbaum, Cullum, 1996

SYMMETRIC INDEFINITE SYSTEM, INDEFINITE PRECONDITIONER

M symmetric indefinite

$$M = M_1 M_2 = M_2^T M_1^T = M^T, \quad M_2 \neq M_1^T$$

M_1, M_2 can be nonsymmetric

$$M_1^{-1} A M_2^{-1} y = M_1^{-1} b, \quad x = M_2^{-1} y$$

$$\tilde{A}\tilde{x} = \tilde{b}, \quad \tilde{A} \text{ nonsymmetric!}$$

ITERATIVE SOLUTION OF (INDEFINITELY) PRECONDITIONED (NONSYMMETRIC) SYSTEM

$$\tilde{A} = M_1^{-1} A M_2^{-1} \; , \qquad \mathcal{J} = M_1^T M_2^{-1}$$

$$\Longrightarrow$$

$$\tilde{A}^T \mathcal{J} = \mathcal{J} \tilde{A}$$

$\mathcal{J}$-SYMMETRIC VARIANT OF (NONSYMMETRIC) LANCZOS PROCESS

Freund, Nachtigal, 1995

SIMPLIFIED $\mathcal{J}$-SYMMETRIC LANCZOS PROCESS AND QMR

$$\tilde{A}^T \mathcal{J} = \mathcal{J} \tilde{A}$$

$$AV_n = V_{n+1} T_{n+1,n}, \; A^T W_n = W_{n+1} \tilde{T}_{n+1,n}$$

$$W_n^T V_n = I \Longrightarrow W_n = \mathcal{J} V_n$$

$\mathcal{J}$-SYMMETRIC VARIANT OF Bi-CG
$\mathcal{J}$-SYMMETRIC VARIANT OF QMR

Freund, Nachtigal, 1995

ITERATIVE SOLUTION OF PRECONDITIONED SYSTEM WITH SIMPLIFIED LANCZOS PROCESS

QMR-from-BiCG:

$$\mathcal{J}\text{-symmetric Bi-CG} + \text{QMR-smoothing}$$
$$\Longrightarrow \mathcal{J}\text{-symmetric QMR}$$

Freund, Nachtigal, 1995

Walker, Zhou 1994

peak/plateau behavior:
QMR does not improve the convergence of Bi-CG (BiCG converges fast $\rightarrow$ QMR is not much better, Bi-CG norm increases $\rightarrow$ quasi-residual of QMR stagnates)

Greenbaum, Cullum, 1996

FINITE PRECISION ARITHMETIC:

smoothing does not improve but also does not deteriorate the rate of primary (unsmoothed Bi-CG) methods (FP analogues for the peak/ plateau property)

smoothing does not improve the final accuracy of the primary method (Bi-CG/QMR on the same level)

Gutknecht, R, 2001

focus on implementation: coupled two-term recursions over the three-term recurrences

Gutknecht, Strakoš, 2000

two-term QMR implementation or two-term Bi-CG + QMR smoothing

SIMPLIFIED Bi-CG ALGORITHM $\Longleftrightarrow$
PRECONDITIONED CG ALGORITHM

$\mathcal{J}$-symmetric Bi-CG algorithm
(classical two-term BI-CG (BIOMIN))

is nothing but

classical (Hestenes-Stiefel) CG algorithm
preconditioned with (indefinite) matrix $\mathcal{J}$!

INDEFINITE SYSTEM, POSITIVE DEFINITE PRECONDITIONER + CONJUGATE GRADIENTS METHOD

Conjugate gradients method: the "symmetrizable" case:

Hageman, Young, 1981

$$(AM^{-1})^T M^{-1} = M^{-1}(AM^{-1})$$

$M^{-1}(AM^{-1})$ and $\mathcal{J} = M^{-1}$ positive definite

Bramble, Pasciak, 1989

Wathen, Stoll, 2007

Liesen, Parlett, 2007

INDEFINITE SYSTEM, INDEFINITE PRECONDITIONER + CLASSICAL CONJUGATE GRADIENTS METHOD

Preconditioned conjugate gradients method (PCG) applied to indefinite system with indefinite preconditioning

is in fact

conjugate gradients method applied to nonsymmetric (and often to non-normal) preconditioned system with AM^{-1}

Nevertheless, it frequently works in practice. Theoretical results?

R, Simoncini, 2002

Andy Wathen?

SADDLE POINT PROBLEM AND INDEFINITE CONSTRAINT PRECONDITIONER

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

$$M = \begin{pmatrix} I & B \\ B^T & 0 \end{pmatrix}$$

PCG method starting with particular right-hand side or initial guess: $\begin{pmatrix} x_0 \\ y_0 \end{pmatrix}, r_0 = \begin{pmatrix} s_0 \\ 0 \end{pmatrix}$

R, Šimoncini, 2002, Gould, Keller, Wathen 2000, Lukšan, Vlček, 1998

SADDLE POINT PROBLEM AND INDEFINITE PRECONDITIONER

$$\begin{pmatrix} A & B \\ B^T & -C \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix}$$

$$M = \begin{pmatrix} A & B \\ B^T & -C + B^T A^{-1} B - D \end{pmatrix}$$

PCG method starting with particular right-hand side and initial guess: $\begin{pmatrix} x_0 \\ 0 \end{pmatrix}, r_0 = \begin{pmatrix} 0 \\ s_0 \end{pmatrix}$

Durazzi, Ruggiero, 2001

SADDLE POINT PROBLEMS: SYMMETRIC INDEFINITE SYSTEMS AND INDEFINITE PRECONDITIONER

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

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

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

INDEFINITE PRECONDITIONER: SPECTRAL PROPERTIES OF PRECONDITIONED SYSTEM

$\mathcal{A}M^{-1}$ **nonsymmetric** and **non-diagonalizable**!

but it has a 'nice' spectrum:

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

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

and only 2 by 2 Jordan blocks!

PRECONDITIONED CG (PCG)

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

$$\begin{pmatrix} x_{k+1} \\ y_{k+1} \end{pmatrix}, \; k = 0, 1, \ldots$$

$$e_{k+1} = \begin{pmatrix} x - x_{k+1} \\ y - y_{k+1} \end{pmatrix}$$

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

BASIC PROPERTIES OF THE CONSTRAINT PRECONDITIONER

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

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

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

THE (ENERGY)-NORM OF ERROR IN PCG

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

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

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

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

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

THE RESIDUAL NORM IN PCG

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

but in general

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

which is reflected in

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

but under appropriate scaling yes!

THE RESIDUAL NORM IN PCG - CONTINUED

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

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

$$\left\| r_{k+1} \right\| = \left\| \phi_{k+1}(A(I - \Pi) + \Pi)s_0 \right\|$$

$$\sigma((I - \Pi)A(I - \Pi)) \subset \sigma(A(I - \Pi) + \Pi)$$

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

$$\Rightarrow \|r_{k+1}\| = \left\| \begin{pmatrix} s_{k+1} \\ 0 \end{pmatrix} \right\| \to 0!$$

SCALING BY A CONSTANT $\alpha > 0$ SUCH THAT

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

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

$$v: \quad \|(I - \Pi)v\| \neq 0$$

$$\alpha = \frac{1}{((I - \Pi)v, A(I - \Pi)v)}!$$

SCALING BY A DIAGONAL?

$$A \rightarrow (diag(A))^{-1/2} A (diag(A))^{-1/2}$$

often gives what we want!

DIFFERENT DIRECTION VECTOR?

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

so that $\|r_{k+1}\| = \|s_{k+1}\|$ is locally minimized!

Braess, Deuflhard,Lipikov 1999, Hribar, Gould, Nocedal, 1999

NUMERICAL EXAMPLE

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

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

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

BEHAVIOR OF PCG IN FINITE PRECISION ARITHMETIC

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

$$\|x - \bar{x}_{k+1}\|_A \leq \gamma_1 \|\Pi(x - \bar{x}_{k+1})\|$$

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

EXACT ARITHMETIC:

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

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

BEHAVIOR OF PCG IN FINITE PRECISION ARITHMETIC

$$\|x - \bar{x}_{k+1}\|_A \leq \gamma_3 \|B^T(x - \bar{x}_{k+1})\|$$

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

DEPARTURE FROM THE NULL-SPACE OF B^T + RESIDUAL PROJECTION ONTO IT

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

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

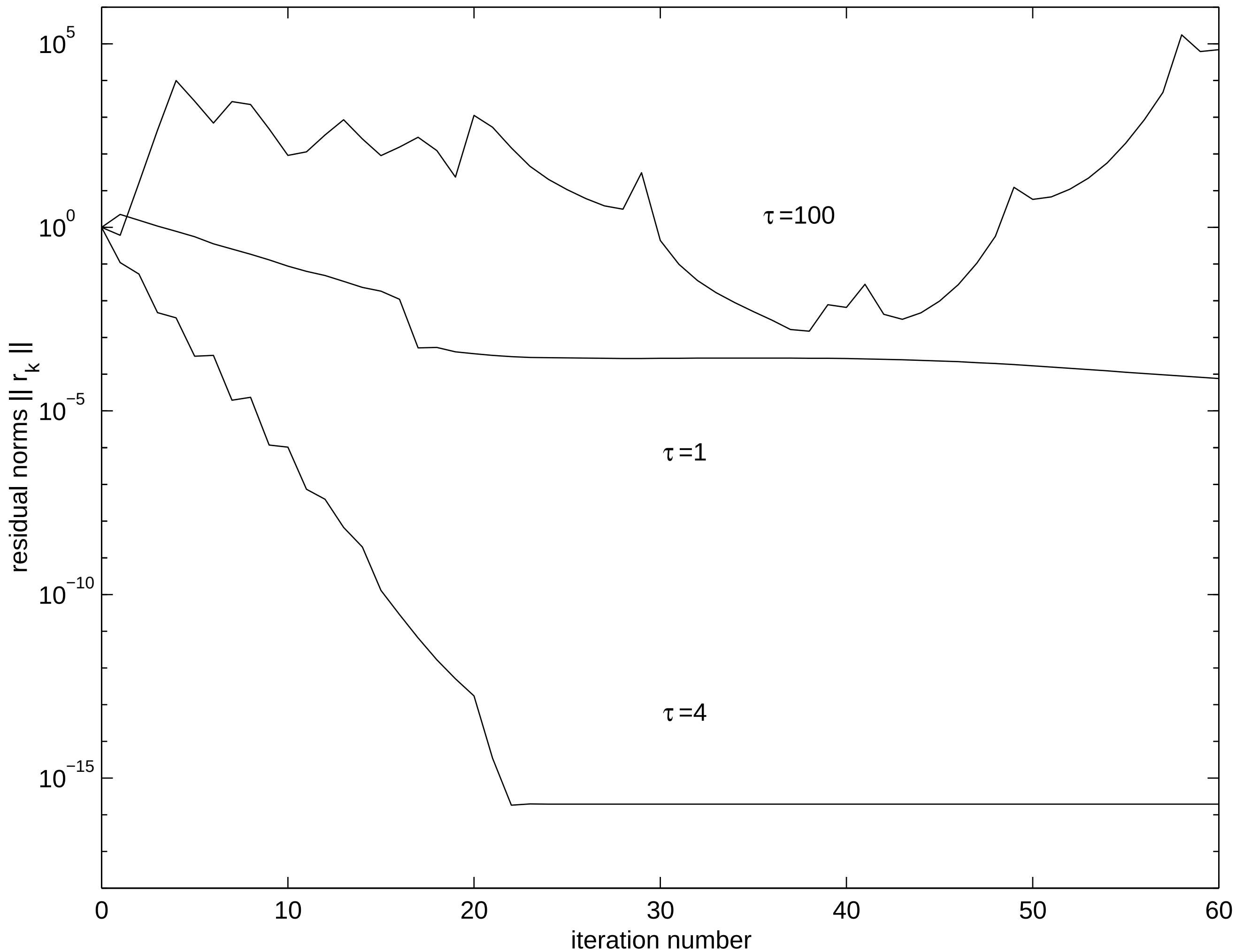
BEHAVIOR OF PCG IN FINITE PRECISION ARITHMETIC

$$\|(f - A\bar{x}_{k+1} - B\bar{y}_{k+1}) - \bar{s}^{(1)}_{k+1}\|,$$
$$\|B^T(x - \bar{x}_{k+1}) - \bar{s}^{(2)}_{k+1}\| \leq$$
$$\leq \| \begin{pmatrix} f \\ 0 \end{pmatrix} - \begin{pmatrix} A & B \\ B^T & 0 \end{pmatrix} \begin{pmatrix} \bar{x}_{k+1} \\ \bar{y}_{k+1} \end{pmatrix} - \begin{pmatrix} \bar{s}^{(1)}_{k+1} \\ \bar{s}^{(2)}_{k+1} \end{pmatrix} \|$$
$$\leq c_1 \varepsilon \kappa(\mathcal{A}) \max_{j=0,\ldots,k+1} \|\bar{r}_j\|$$

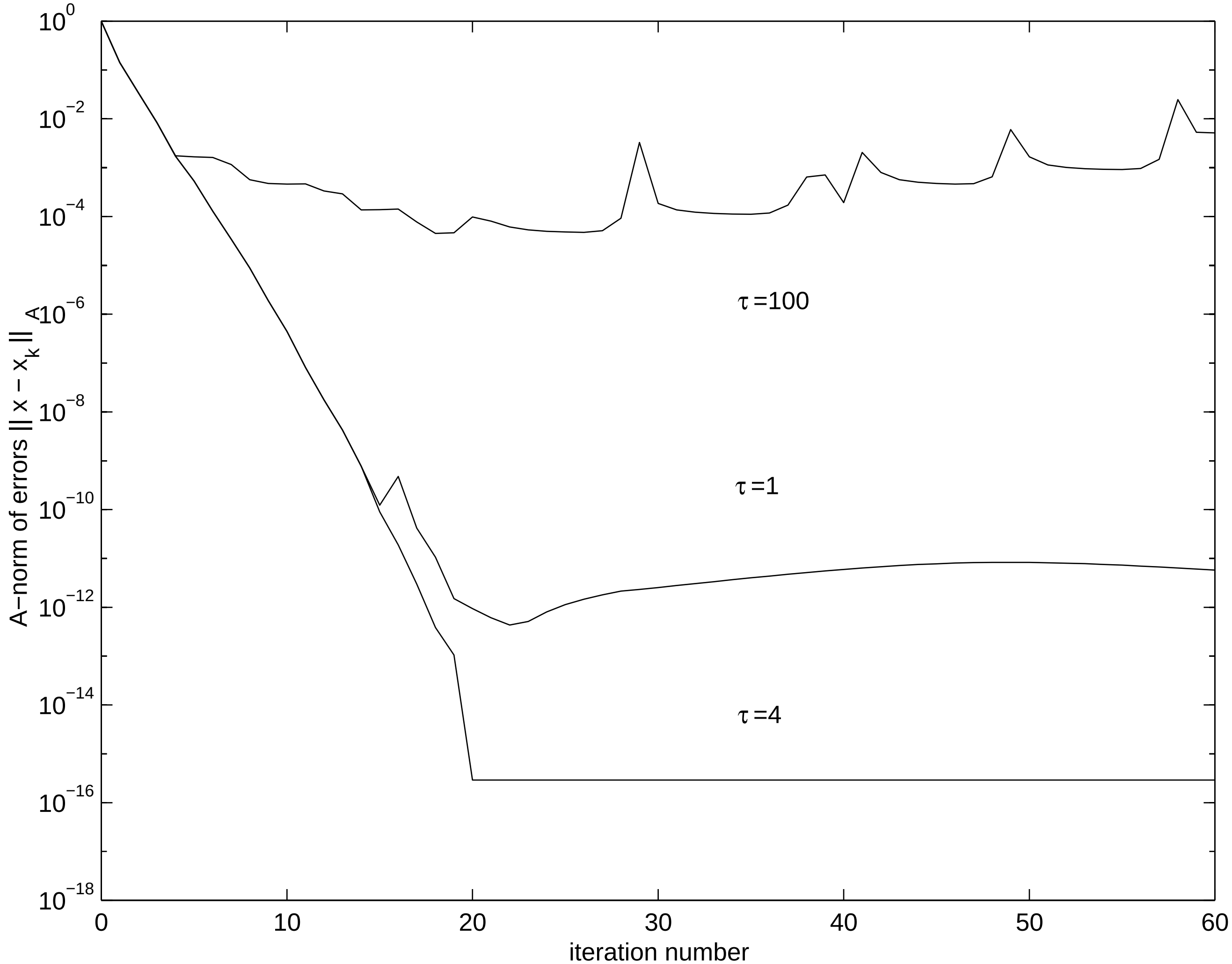
Greenbaum 1994,1997, Sleijpen, et al. 1994

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

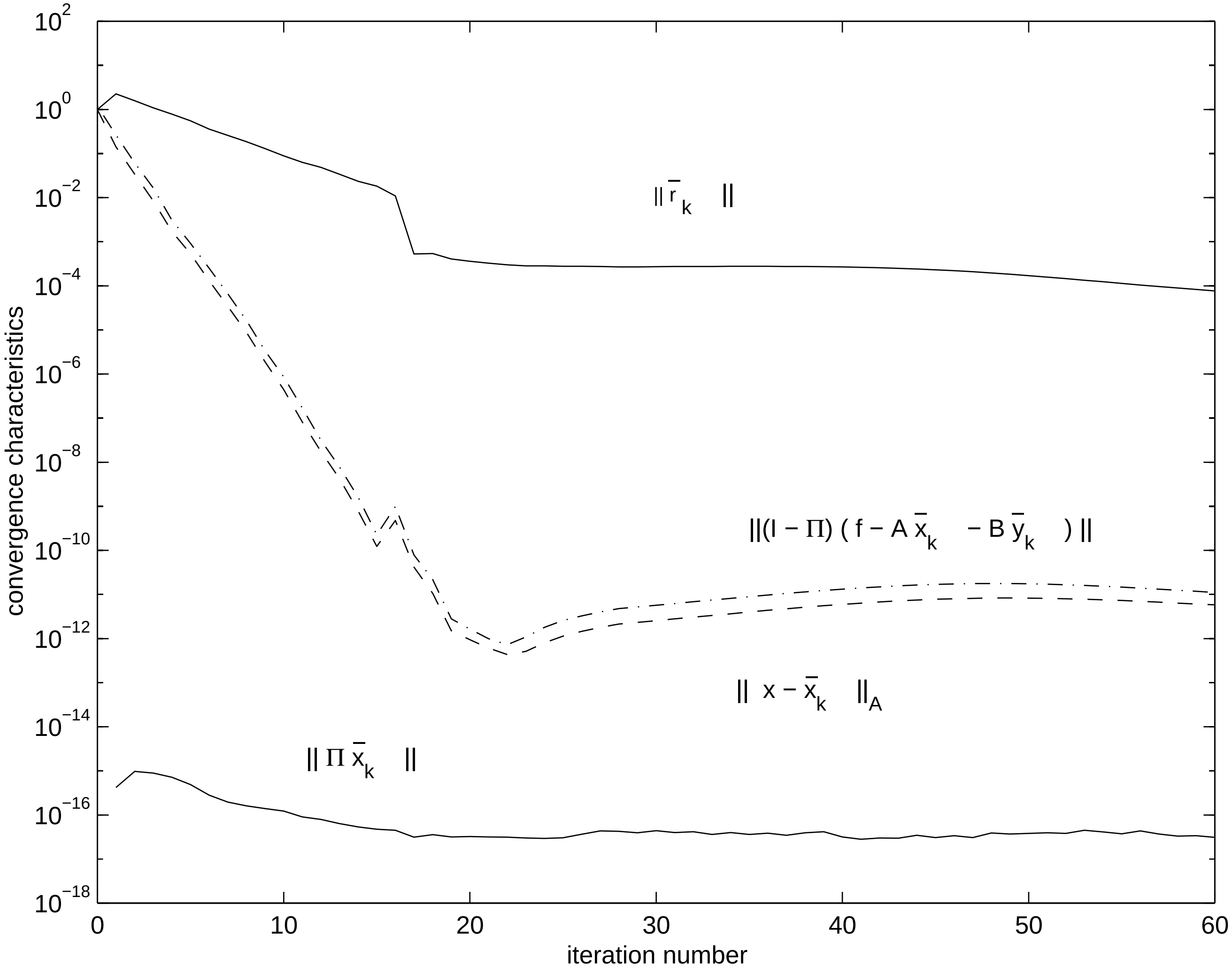
$$\|\bar{r}_0\| \sim \max_{j=0,\ldots,k+1} \|\bar{r}_j\|$$

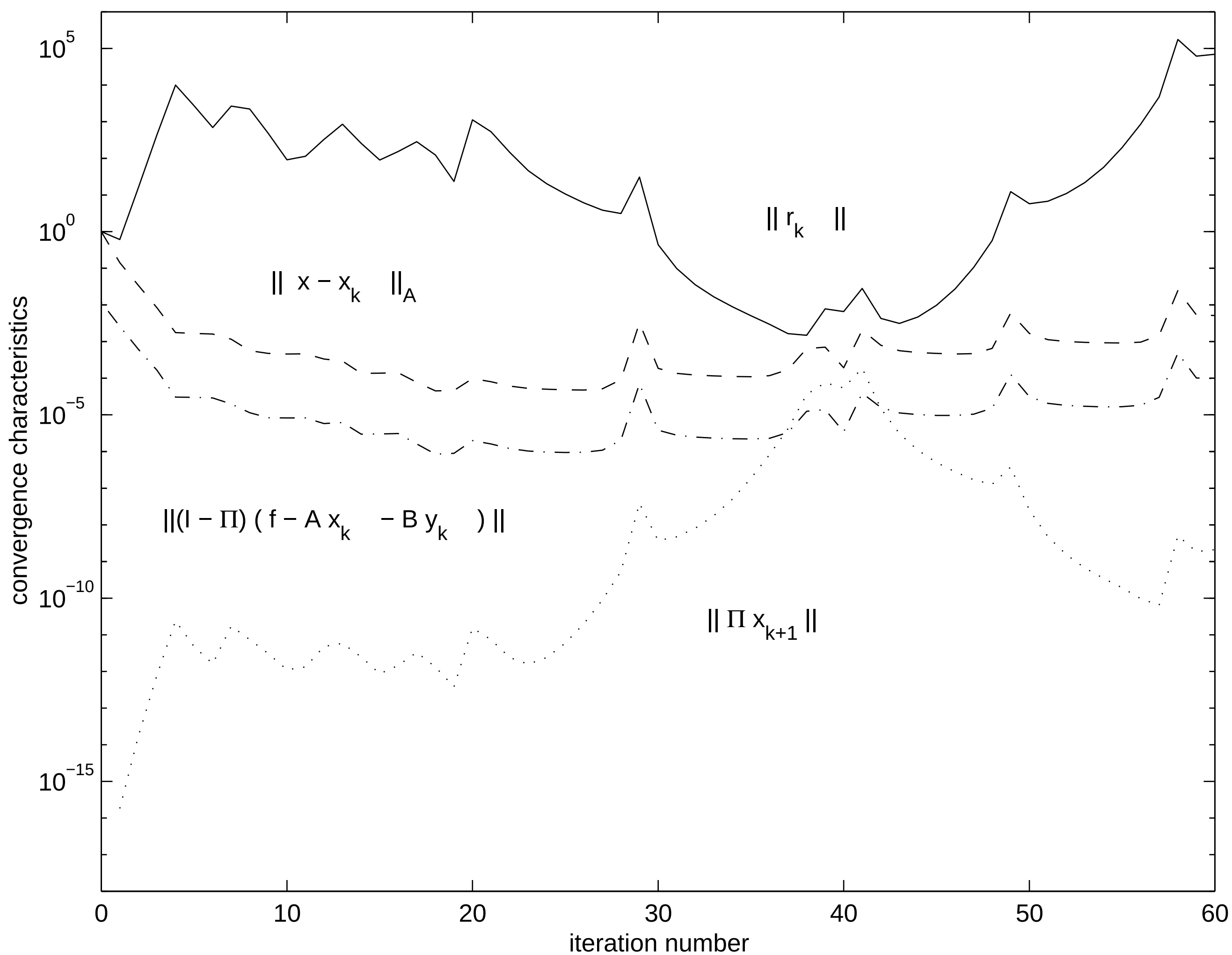


10^5
10^0
10^{-5}
10^{-10}
10^{-15}
residual norms $\| r_k \|$
$\tau = 100$
$\tau = 1$
$\tau = 4$
0
10
20
30
40
50
60
iteration number

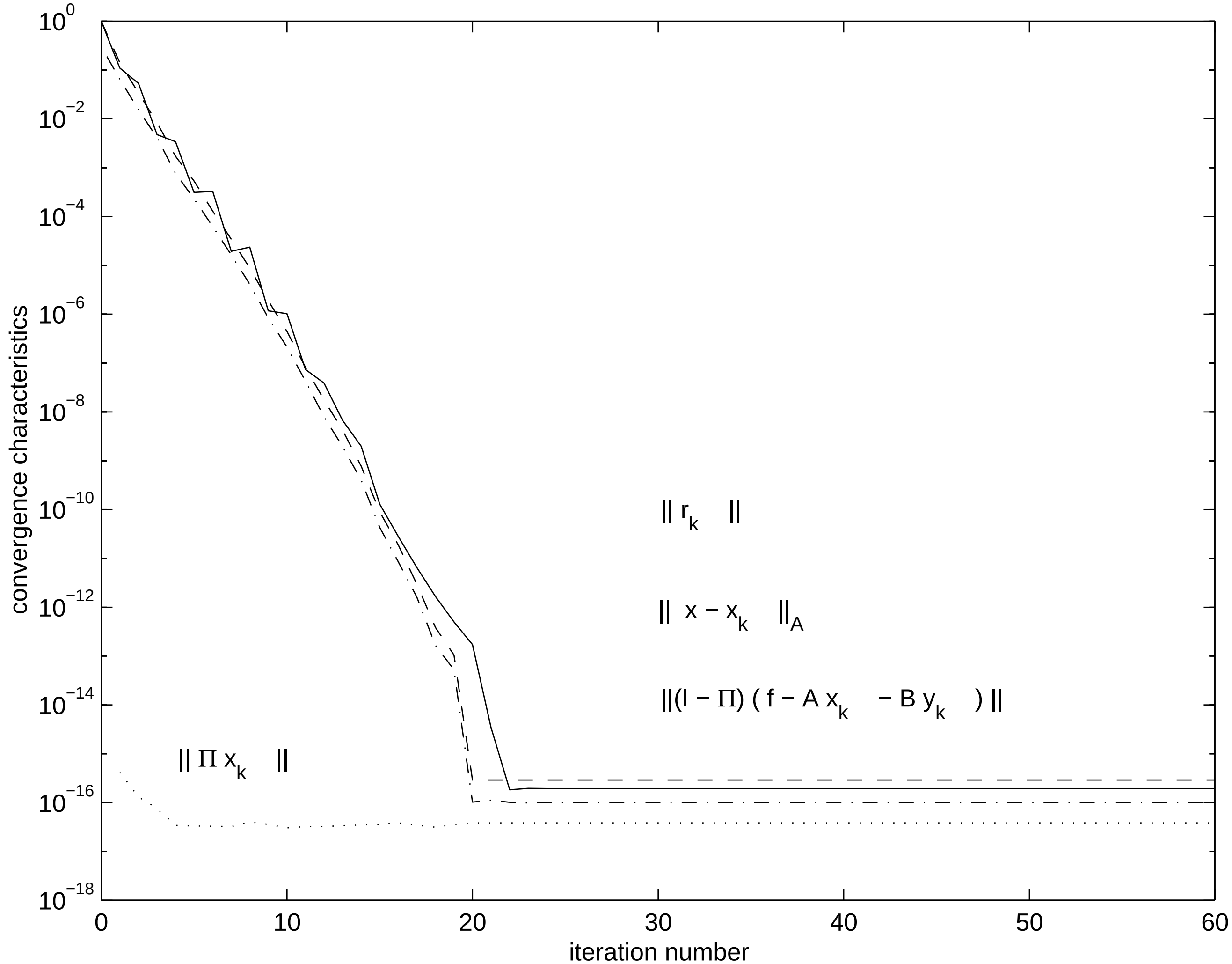


10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}
10^{-16}
10^{-18}
A−norm of errors $\|x - x_k\|_A$
$\tau = 100$
$\tau = 1$
$\tau = 4$
0
10
20
30
40
50
60
iteration number


convergence characteristics
iteration number
$\| \bar{r}_k \|$
$\|(I - \Pi)(f - A\bar{x}_k - B\bar{y}_k)\|$
$\| x - \bar{x}_k \|_A$
$\| \Pi \bar{x}_k \|$



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



convergence characteristics
iteration number
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
$\| r_k \|$
$\| x - x_k \|_A$
$\|(I - \Pi) (f - A x_k - B y_k)\|$
$\| \Pi x_k \|$

THANK YOU FOR YOUR ATTENTION!