

THE CONJUGATE GRADIENTS METHOD WITH INDEFINITE PRECONDITIONING

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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 \iff 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

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

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

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

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

\implies

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

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

Freund, Nachtigal, 1995

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

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

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

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

\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} -symmetric Bi-CG + QMR-smoothing
 $\implies \mathcal{J}$ -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 \iff
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, INDEFINITE PRECONDITIONER + CLASSICAL CONJUGATE GRADIENTS METHODS

Preconditioned conjugate gradients methods (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, 2001

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, Simoncini, 2001, Gould et al., 2000

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 $\text{span}(B)$

INDEFINITE PRECONDITIONER: SPECTRAL PROPERTIES OF PRECONDITIONED SYSTEM

AM^{-1} nonsymmetric and non-diagonalizable!

but it has a 'nice' spectrum:

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

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

and only 2 by 2 Jordan blocks!

PRECONDITIONED CG (PCG)

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

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

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

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

BASIC PROPERTIES OF THE CONSTRAINT PRECONDITIONER

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

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

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

THE (ENERGY)-NORM OF ERROR IN PCG

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

SCALING BY A DIAGONAL?

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

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, Deufhard, Lipikov 1999, Hribar, Gould, Nocedal, 1999

NUMERICAL EXAMPLE

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

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

$$\alpha \quad \sigma\left(\begin{pmatrix} \alpha A & B \\ B^T & 0 \end{pmatrix} \begin{pmatrix} I & B \\ B^T & 0 \end{pmatrix}^{-1}\right)$$

1/100	[0.0207, 0.0586]	{1}
1/10	[0.2067, 0.5856]	{1}
1/4	[0.5170, 1.4641]	
1	{1}	[2.0678, 5.8563]
4	{1}	[8.2712, 23.4252]

BEHAVIOR OF PCG IN FINITE PRECISION ARITHMETIC

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

$$\begin{aligned} \|x - \bar{x}_{k+1}\|_A &\leq \gamma_1 \|\Pi(x - \bar{x}_{k+1})\| \\ &+ \gamma_2 \|(I - \Pi)A(I - \Pi)(x - \bar{x}_{k+1})\| \end{aligned}$$

EXACT ARITHMETIC:

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

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

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

$$B^T(x - \bar{x}_{k+1}) \sim \bar{s}_{k+1}^{(2)} \\ (I - \Pi)(f - A\bar{x}_{k+1} - B\bar{y}_{k+1}) \sim (I - \Pi)\bar{s}_{k+1}^{(1)}$$

BEHAVIOR OF PCG IN FINITE PRECISION ARITHMETIC

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

Greenbaum 1994,1997, Sleijpen, et al. 1994

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

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









