

GMRES Methods for Least Squares Problems

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Problem:

$$\min_{\mathbf{x} \in \mathbf{R}^n} \|\mathbf{b} - A\mathbf{x}\|_2$$

$$A \in \mathbf{R}^{m \times n}$$

- $m > n$ or $m = n$ or $m < n$
- not necessarily full rank
- large sparse



$$A^T A \mathbf{x} = A^T \mathbf{b} \quad (\text{normal equation})$$

For $m < n$

$$AA^T \mathbf{y} = \mathbf{b}, \quad \mathbf{x} = A^T \mathbf{y}$$



minimum norm solution

1. Iterative methods using the normal equation

$A^T A$: square, symmetric,
positive definite (if $\text{rank} A = n$) matrix



Apply Conjugate Gradient method.



CGLS (Conjugate Gradient Least Squares) method

The CGLS(CGNR) method

Choose x_0 .

$$r_0 = b - Ax_0, \quad p_0 = s_0 = A^T r_0, \quad \gamma_0 = \|s_0\|_2^2$$

for $i = 0, 1, 2, \dots$ until $\gamma_i < \epsilon$

$$q_i = Ap_i$$

$$\alpha_i = \gamma_i / \|q_i\|_2^2$$

$$x_{i+1} = x_i + \alpha_i p_i$$

$$r_{i+1} = r_i - \alpha_i q_i$$

$$s_{i+1} = A^T r_{i+1}$$

$$\gamma_{i+1} = \|s_{i+1}\|_2^2$$

$$\beta_i = \gamma_{i+1} / \gamma_i$$

$$p_{i+1} = s_{i+1} + \beta_i p_i$$

endfor

However,

condition number of $A^T A$: square of A .



Slow convergence

Preconditioning necessary

- diagonal scaling
- incomplete Cholesky decomposition
(Meijerink, van der Vorst '77)
- incomplete QR decomposition
(Jennings, Ajiz '84, Saad '88)
- incomplete Givens orthogonalization
(Bai et al. '01)
- robust incomplete factorization (RIF)
(Benzi, Tuma '03)

etc.

2. Iterative methods not based on the normal equation

CR-LS(k) method (Zhang and Oyanagi, '89)

Apply Orthomin(k) method to

$$\min_{\mathbf{x} \in \mathbf{R}^n} \|\mathbf{b} - A\mathbf{x}\|_2$$

by introducing a mapping matrix $B \in \mathbf{R}^{n \times m}$,
and using the Krylov subspace generated by
 $AB \in \mathbf{R}^{m \times m}$.

Consider using
GMRES (Generalized Minimal RESidual) method
instead.

GMRES: efficient and robust method for

$$Ax = b,$$

where

$A \in \mathbf{R}^{n \times n}$: nonsingular.

GMRES(k) method

Choose x_0

* $r_0 = b - Ax_0$; $v_1 = r_0 / \|r_0\|_2$

for $i = 1, 2, \dots, k$

$$w_i = Av_i$$

for $j = 1, 2, \dots, i$

$$h_{j,i} = (w_i, v_j)$$

$$w_i = w_i - h_{j,i}v_j$$

end for

$$h_{i+1,i} = \|w_i\|_2$$

$$v_{i+1} = w_i / h_{i+1,i}$$

Find $y_i \in \mathbf{R}^i$ which minimizes $\|r_i\|_2 = \| \|r_0\|_2 e_i - \bar{H}_i y \|_2$.

if $\|r_i\|_2 < \epsilon$ then

$$x_i = x_0 + [v_1, \dots, v_i]y_i; \text{ stop}$$

endif

endfor

$$x_k = x_0 + [v_1, \dots, v_k]y_k$$

$$x_0 = x_k$$

Go to *.

(Here, $\bar{H}_i = (h_{pq}) \in \mathbf{R}^{(i+1) \times i}$,
 $e_i = (1, 0, \dots, 0)^\top \in \mathbf{R}^{i+1}$.)

Minimizes $\|\mathbf{r}_k\|_2$ over

$$\begin{aligned}\mathbf{x}_k &= \mathbf{x}_0 + \langle \mathbf{v}_1, \dots, \mathbf{v}_k \rangle \\ \langle \mathbf{v}_1, \dots, \mathbf{v}_k \rangle &= \langle \mathbf{r}_0, A\mathbf{r}_0, \dots, A^{k-1}\mathbf{r}_0 \rangle \\ (\mathbf{v}_i, \mathbf{v}_j) &= \delta_{ij}\end{aligned}$$

$k = \infty$: (full) GMRES.

$h_{i+1,i} = 0$: breakdown

When A : nonsingular,

GMRES does not break down until it has found the solution of $A\mathbf{x} = \mathbf{b}$, $\forall \mathbf{b}, \forall \mathbf{x}_0 \in \mathbf{R}^n$ (with in n steps).

When A : singular,

Theorem 1 (*Brown, Walker '97*)

GMRES determines a least squares solution of $\min_{\mathbf{x} \in \mathbf{R}^n} \|\mathbf{b} - A\mathbf{x}\|_2$ without breakdown $\forall \mathbf{b}, \forall \mathbf{x}_0 \in \mathbf{R}^n$

$$\begin{array}{c} \Updownarrow \\ \mathcal{R}(A) = \mathcal{R}(A^T). \quad \square \end{array}$$

$\mathcal{R}(M)$: range space of M .

How can we apply GMRES to
the least squares problem

$$\min_{\mathbf{x} \in \mathbf{R}^n} \|\mathbf{b} - A\mathbf{x}\|_2$$

where $A \in \mathbf{R}^{m \times n}$?

$$A \in \mathbf{R}^{m \times n}, \quad \mathbf{r}_0 = \mathbf{b} - A\mathbf{x}_0 \in \mathbf{R}^m.$$

↓

Cannot create Krylov subspace by $A \times \mathbf{r}_0$.

Basically two ways to overcome

by using a mapping matrix $B \in \mathbf{R}^{n \times m}$.

1. AB-GMRES method

Use Krylov subspace:

$$\mathcal{K}_k(AB, \mathbf{r}_0) := \langle \mathbf{r}_0, AB\mathbf{r}_0, \dots, (AB)^{i-1}\mathbf{r}_0 \rangle \text{ in } \mathbf{R}^m.$$

$$AB \in \mathbf{R}^{m \times m}.$$

(cf. CR-LS(k) method by Zhang, Oyanagi)

First note:

Lemma 2

$$\min_{\mathbf{x} \in \mathbf{R}^n} \|\mathbf{b} - A\mathbf{x}\|_2 = \min_{\mathbf{z} \in \mathbf{R}^m} \|\mathbf{b} - AB\mathbf{z}\|_2 \quad \forall \mathbf{b} \in \mathbf{R}^m$$

\Leftrightarrow

$$\mathcal{R}(A) = \mathcal{R}(AB) \quad \square$$

Using

Lemma 3 $\mathcal{R}(AA^T) = \mathcal{R}(A)$ \square

we can show

Lemma 4 $\mathcal{R}(A^T) = \mathcal{R}(B) \implies \mathcal{R}(A) = \mathcal{R}(AB)$. \square

Thus, assume $\mathcal{R}(A) = \mathcal{R}(AB)$.

Consider solving

$$\min_{\mathbf{z} \in \mathbf{R}^m} \|\mathbf{b} - AB\mathbf{z}\|_2 = \min_{\mathbf{x} \in \mathbf{R}^n} \|\mathbf{b} - A\mathbf{x}\|_2$$

using GMRES with initial approximation

$$\mathbf{z}_0 \in \mathbf{R}^m; \quad AB\mathbf{z}_0 = A\mathbf{x}_0.$$

Then, we have the following.

AB-GMRES(k) method

Choose x_0 ($; Ax_0 = ABz_0$).

* $r_0 = b - Ax_0$ ($= b - ABz_0$); $v_1 = r_0 / \|r_0\|_2$

for $i = 1, 2, \dots, k$

$$w_i = ABv_i$$

for $j = 1, 2, \dots, i$

$$h_{j,i} = (w_i, v_j)$$

$$w_i = w_i - h_{j,i}v_j$$

end for

$$h_{i+1,i} = \|w_i\|_2$$

$$v_{i+1} = w_i / h_{i+1,i}$$

Find $y_i \in \mathbf{R}^i$ which minimizes $\|r_i\|_2 = \| \|r_0\|_2 e_i - \bar{H}_i y \|_2$

$$x_i = x_0 + B[v_1, \dots, v_i]y_i$$

$$r_i = b - Ax_i$$

if $\|A^T r_i\|_2 < \epsilon$ stop

endfor

$$x_0 = x_k$$

Go to *.

Does the AB-GMRES method determine the least squares solution without breakdown ?

Recall the following.

Theorem 5 (*Brown, Walker '97*)

Let $\tilde{A} \in \mathbf{R}^{m \times m}$. Then, the following holds.

The GMRES method determines

a least squares solution of $\min_{z \in \mathbf{R}^m} \|\mathbf{b} - \tilde{A}z\|_2$

$\forall \mathbf{b} \in \mathbf{R}^m, \forall z_0 \in \mathbf{R}^m$ without breakdown

\Updownarrow

$$\mathcal{R}(\tilde{A}) = \mathcal{R}(\tilde{A}^\top). \quad \square$$

Let $\tilde{A} := AB$. Noting

Theorem 6 *If $\mathcal{R}(A^\top) = \mathcal{R}(B)$, then*

$$\mathcal{R}(AB) = \mathcal{R}(B^\top A^\top) \iff \mathcal{R}(A) = \mathcal{R}(B^\top) \quad \square$$

we obtain

Theorem 7

If $\mathcal{R}(A^\top) = \mathcal{R}(B)$, then

AB-GMRES method determines

a least squares solution of $\min_{\mathbf{x} \in \mathbf{R}^n} \|\mathbf{b} - A\mathbf{x}\|_2$

$\forall \mathbf{b} \in \mathbf{R}^m, \forall \mathbf{x}_0 \in \mathbf{R}^n$ without breakdown

\Updownarrow

$$\mathcal{R}(A) = \mathcal{R}(B^\top). \quad \square$$

Corollary 8

$$\mathcal{R}(A^\top) = \mathcal{R}(B), \quad \mathcal{R}(A) = \mathcal{R}(B^\top)$$



AB-GMRES method determines

a least squares solution of $\min_{\mathbf{x} \in \mathbf{R}^n} \|\mathbf{b} - A\mathbf{x}\|_2$

$\forall \mathbf{b} \in \mathbf{R}^m, \forall \mathbf{x}_0 \in \mathbf{R}^n$ without breakdown. \square

Remark 1

$$\mathcal{R}(A) = \mathcal{R}(B^\top)$$



$$B^\top = AC^\top; \quad C^\top: \text{nonsingular}$$



$$B = CA^\top; \quad C: \text{nonsingular.}$$

2. BA-GMRES method

The other alternative:

Use a matrix $B \in \mathbf{R}^{n \times m}$
to map $\mathbf{r}_0 \in \mathbf{R}^m$ to $\tilde{\mathbf{r}}_0 = B\mathbf{r}_0 \in \mathbf{R}^n$.

Then create Krylov subspace

$$\langle \tilde{\mathbf{r}}_0, BA\tilde{\mathbf{r}}_0, \dots, (BA)^{i-1}\tilde{\mathbf{r}}_0 \rangle \text{ in } \mathbf{R}^n.$$

$$BA \in \mathbf{R}^{n \times n}$$

First note:

Theorem 9

$$\|\mathbf{b} - A\mathbf{x}^*\|_2 = \min_{\mathbf{x} \in \mathbf{R}^n} \|\mathbf{b} - A\mathbf{x}\|_2$$

and

$$\|B\mathbf{b} - BA\mathbf{x}^*\|_2 = \min_{\mathbf{x} \in \mathbf{R}^n} \|B\mathbf{b} - BA\mathbf{x}\|_2$$

are equivalent for all $\mathbf{b} \in \mathbf{R}^m$



$$\mathcal{R}(A) = \mathcal{R}(B^T BA).$$

Also note

Lemma 10

$$\mathcal{R}(A) = \mathcal{R}(B^\top) \implies \mathcal{R}(BA) = \mathcal{R}(B).$$

Lemma 11

$$\mathcal{R}(BA) = \mathcal{R}(B) \implies \mathcal{R}(B^\top BA) = \mathcal{R}(B^\top).$$

Lemma 12

$$\mathcal{R}(A) = \mathcal{R}(B^\top) \implies \mathcal{R}(A) = \mathcal{R}(B^\top BA).$$

Thus, assume $\mathcal{R}(A) = \mathcal{R}(B^\top BA)$,

and consider applying GMRES(k) method to

$$\min_{\mathbf{x} \in \mathbf{R}^n} \|B\mathbf{b} - BA\mathbf{x}\|_2$$

with initial approximation \mathbf{x}_0 .

BA-GMRES(k) method

Choose x_0 .

$$* \tilde{r}_0 = B(\mathbf{b} - A\mathbf{x}_0)$$

$$\mathbf{v}_1 = \tilde{r}_0 / \|\tilde{r}_0\|_2$$

for $i = 1, 2, \dots, k$ until convergence

$$\mathbf{w}_i = BA\mathbf{v}_i$$

for $j = 1, 2, \dots, i$

$$h_{j,i} = (\mathbf{w}_i, \mathbf{v}_j)$$

$$\mathbf{w}_i = \mathbf{w}_i - h_{j,i}\mathbf{v}_j$$

end for

$$h_{i+1,i} = \|\mathbf{w}_i\|_2$$

$$\mathbf{v}_{i+1} = \mathbf{w}_i / h_{i+1,i}$$

Find $\mathbf{y}_i \in \mathbf{R}^i$ which minimizes $\|\tilde{r}_i\|_2 = \|\|\tilde{r}_0\|_2 \mathbf{e}_i - \bar{H}_i \mathbf{y}\|_2$

$$\mathbf{x}_i = \mathbf{x}_0 + [\mathbf{v}_1, \dots, \mathbf{v}_i] \mathbf{y}_i$$

$$\mathbf{r}_i = \mathbf{b} - A\mathbf{x}_i$$

if $\|A^T \mathbf{r}_i\|_2 < \epsilon$ stop

end for

Go to *.

Does BA-GMRES method give the least squares solution without breakdown ?

Noting

Theorem 13 *If $\mathcal{R}(A) = \mathcal{R}(B^\top)$, then*

$$\mathcal{R}(BA) = \mathcal{R}(A^\top B^\top) \iff \mathcal{R}(A^\top) = \mathcal{R}(B). \quad \square$$

Theorem 14

If $\mathcal{R}(A) = \mathcal{R}(B^\top)$, then

BA-GMRES method determines

a least squares solution of $\min_{\mathbf{x} \in \mathbf{R}^m} \|\mathbf{b} - A\mathbf{x}\|_2$

$\forall \mathbf{b} \in \mathbf{R}^m, \forall \mathbf{x}_0 \in \mathbf{R}^n$ without breakdown



$\mathcal{R}(A^\top) = \mathcal{R}(B)$. \square

Corollary 15

$\mathcal{R}(A) = \mathcal{R}(B^\top), \mathcal{R}(A^\top) = \mathcal{R}(B)$



BA-GMRES method determines

a least squares solution of $\min_{\mathbf{x} \in \mathbf{R}^m} \|\mathbf{b} - A\mathbf{x}\|_2$

$\forall \mathbf{b} \in \mathbf{R}^m, \forall \mathbf{x}_0 \in \mathbf{R}^n$ without breakdown. \square

Summary on condition for B

General case: $\text{rank}A \leq \min(m, n)$,

$$\mathcal{R}(A) = \mathcal{R}(B^T), \quad \mathcal{R}(A^T) = \mathcal{R}(B)$$

↓

AB-GMRES, BA-GMRES methods give
a least squares solution of $\min_{\mathbf{x} \in \mathbf{R}^m} \|\mathbf{b} - A\mathbf{x}\|_2$

$\forall \mathbf{b} \in \mathbf{R}^m, \forall \mathbf{x}_0 \in \mathbf{R}^n$ without breakdown.

... e.g. Let $B = \alpha A^T$ where $0 \neq \alpha \in \mathbf{R}$.

Full rank case

$m \geq n = \text{rank}A$ (over-determined case)

Let $B = CA^T$ where $C \in \mathbf{R}^{n \times n}$: nonsingular
($B, A^T \in \mathbf{R}^{n \times m}$).

\Downarrow

$$B^T = AC^T$$

\Downarrow

$$\mathcal{R}(A) = \mathcal{R}(B^T).$$

\Downarrow

$$n = \text{rank}A^T = \text{rank}A = \text{rank}B^T = \text{rank}B$$

\Downarrow

$$\mathcal{R}(A^T) = \mathcal{R}(B) = \mathbf{R}^n.$$

Since $AB \in \mathbf{R}^{m \times m}$, $BA \in \mathbf{R}^{n \times n}$, $m \geq n$,

use BA-GMRES method.

e.g. Let $C := \{\text{diag}(A^T A)\}^{-1}$

i.e. $BA = \{\text{diag}(A^T A)\}^{-1} A^T A$.

Convergence Analysis

Theorem 16 *Let $A \in \mathbf{R}^{m \times n}$, $m \geq n$,
 $B := CA^T$, $C \in \mathbf{R}^{n \times n}$: sym.pos.def.,
 σ_i ($1 \leq i \leq n$): singular values of $\tilde{A} := AC^{\frac{1}{2}}$.
Then,
 σ_i^2 ($1 \leq i \leq n$) : eigenvalues of AB and BA .
If $m > n$, all other eigenvalues of AB are 0.*

[Proof]

Let $\tilde{A} := AC^{\frac{1}{2}} = U\Sigma V^{\top}$: SVD,

$U \in \mathbf{R}^{m \times m}, V \in \mathbf{R}^{n \times n}$: orthogonal matrices,

$$\Sigma = \begin{bmatrix} \sigma_1 & & & 0 \\ & \dots & & \\ & & \sigma_n & \\ 0 & & & \end{bmatrix} \in \mathbf{R}^{m \times n},$$

$\sigma_1 \geq \dots \geq \sigma_n \geq 0$: singular values of \tilde{A} .

Then,

$$AB = ACA^{\top} = \tilde{A}\tilde{A}^{\top} = U\Sigma\Sigma^{\top}U^{\top},$$

$$BA = CA^{\top}A = C^{\frac{1}{2}}\tilde{A}^{\top}\tilde{A}C^{-\frac{1}{2}} = C^{\frac{1}{2}}V\Sigma^{\top}\Sigma(C^{\frac{1}{2}}V)^{-1}. \quad \blacksquare$$

cf. If $\text{rank}A = n$, $C := \{\text{diag}(A^{\top}A)\}^{-1}$: sym.pos.def.

Similarly for RIF.

Theorem 17 *The residual $\mathbf{r} = \mathbf{b} - A\mathbf{x}$ achieved by the k -th step of AB-GMRES satisfies*

$$\|\mathbf{r}_k|_{\mathcal{R}(A)}\|_2 \leq 2 \left(\frac{\sigma_1 - \sigma_n}{\sigma_1 + \sigma_n} \right)^k \|\mathbf{r}_0|_{\mathcal{R}(A)}\|_2. \quad \blacksquare$$

Theorem 18 *The residual $\mathbf{r} = \mathbf{b} - A\mathbf{x}$ achieved by the k -th step of BA-GMRES satisfies*

$$\|B\mathbf{r}_k\|_2 = \|CA^\top \mathbf{r}_k\|_2 \leq 2\sqrt{\kappa(C)} \left(\frac{\sigma_1 - \sigma_n}{\sigma_1 + \sigma_n} \right)^k \|B\mathbf{r}_0\|_2. \quad \blacksquare$$

CGLS method

Preconditionings

$$LDL^T \sim A^T A, \tilde{L} = LD^{\frac{1}{2}} \text{ (e.g. RIF)}$$

$$\text{diag}(A^T A) \sim A^T A, \tilde{L} = (\text{diag}(A^T A))^{\frac{1}{2}}.$$

Apply CG to

$$A'x' = b' \quad (*)$$

where

$$A' = \tilde{L}^{-1} A^T A \tilde{L}^{-T}$$

$$x' = \tilde{L}^T x$$

$$b = \tilde{L}^{-1} A^T b.$$

Since

$$(\tilde{L}^\top)^{-1} A' (\tilde{L}^\top) = C A^\top A = BA,$$

$$\lambda_i(A') = \lambda_i(BA) = \sigma_i^2, \quad i = 1, \dots, n$$

Theorem 19 *The residual $\mathbf{r} = \mathbf{b} - A\mathbf{x}$ of the k -th step of preconditioned CGLS (CG applied to $(*)$) satisfies*

$$\|A^\top \mathbf{r}_k\|_{(A^\top A)^{-1}} = \|e_m\|_{A^\top A} \leq 2 \left(\frac{\sigma_1 - \sigma_n}{\sigma_1 + \sigma_n} \right)^k \|A^\top \mathbf{r}_0\|_{(A^\top A)^{-1}}. \quad \blacksquare$$

Similar convergence behaviours expected for
AB-GMRES, BA-GMRES,
and preconditioned CGLS methods,
using the same preconditioner C .

rank $A = m \leq n$ (under-determined case)

Let $B = A^T C$ where $C \in \mathbf{R}^{m \times m}$: nonsingular
($B, A^T \in \mathbf{R}^{n \times m}$).

\Downarrow

$$\mathcal{R}(A^T) = \mathcal{R}(B).$$

\Downarrow

$$m = \text{rank}A = \text{rank}A^T = \text{rank}B = \text{rank}B^T$$

\Downarrow

$$\mathcal{R}(A) = \mathcal{R}(B^T) = \mathbf{R}^m.$$

Since $AB \in \mathbf{R}^{m \times m}$, $BA \in \mathbf{R}^{n \times n}$, $m \leq n$,
use AB-GMRES method.

e.g. Let $C := \{\text{diag}(AA^T)\}^{-1}$.

i.e. $AB = AA^T \{\text{diag}(AA^T)\}^{-1}$.

Note that when $\text{rank}A = m$, $\mathcal{R}(A) = \mathbf{R}^m \ni \mathbf{b}$,
so that

$$\min_{\mathbf{x} \in \mathbf{R}^n} \|\mathbf{b} - A\mathbf{x}\| = \min_{\mathbf{z} \in \mathbf{R}^m} \|\mathbf{b} - AB\mathbf{z}\| = \min_{\mathbf{z} \in \mathbf{R}^m} \|\mathbf{b} - AA^T C\mathbf{z}\| = 0.$$

Hence, AB-GMRES method with $B = A^T C$
gives the minimum norm least squares
solution

$$\mathbf{x}^* = B\mathbf{z}^* = A^T(C\mathbf{z}^*)$$

of

$$\min_{\mathbf{x} \in \mathbf{R}^n} \|\mathbf{b} - A\mathbf{x}\|$$

since

$$AA^T(C\mathbf{z}^*) = \mathbf{b}.$$

Theorem 20

Let $A \in \mathbf{R}^{m \times n}$, $m \leq n$,

$B := A^T C$, $C \in \mathbf{R}^{m \times m}$: sym.pos.def.,

σ_i ($1 \leq i \leq m$): singular values of $\tilde{A} := C^{\frac{1}{2}} A$.

Then,

σ_i^2 ($1 \leq i \leq m$) : eigenvalues of AB and BA .

If $m < n$, all other eigenvalues of BA are 0.

[Proof]

Let $\tilde{A} := C^{\frac{1}{2}}A = U\Sigma V^T$: SVD,

$U \in \mathbf{R}^{m \times m}, V \in \mathbf{R}^{n \times n}$: orthogonal matrices,

$$\Sigma = \begin{bmatrix} \sigma_1 & & & 0 \\ & \dots & & \\ & & \sigma_m & \\ & & & \end{bmatrix} \in \mathbf{R}^{m \times n},$$

$\sigma_1 \geq \dots \geq \sigma_m \geq 0$: singular values of \tilde{A} .

Then,

$$AB = AA^T C = C^{-\frac{1}{2}} \tilde{A} \tilde{A}^T C^{\frac{1}{2}} = C^{-\frac{1}{2}} U \Sigma \Sigma^T (C^{-\frac{1}{2}} U)^{-1},$$

$$BA = A^T C A = \tilde{A}^T \tilde{A} = V \Sigma^T \Sigma V^T. \quad \blacksquare$$

cf. If $\text{rank} A = m$,

$C := \{\text{diag}(AA^T)\}^{-1}$: sym.pos.def.

Similarly for RIF.

Theorem 21 *The residual $\mathbf{r} = \mathbf{b} - A\mathbf{x}$ achieved by the k -th step of AB-GMRES satisfies*

$$\|\mathbf{r}_k\|_2 \leq 2\sqrt{\kappa_2(C)} \left(\frac{\sigma_1 - \sigma_m}{\sigma_1 + \sigma_m} \right)^k \|\mathbf{r}_0\|_2. \quad \blacksquare$$

Theorem 22 *The residual $\mathbf{r} = \mathbf{b} - A\mathbf{x}$ achieved by the k -th step of BA-GMRES satisfies*

$$\|B\mathbf{r}_k|_{\mathcal{R}(B)}\|_2 \leq 2 \left(\frac{\sigma_1 - \sigma_m}{\sigma_1 + \sigma_m} \right)^k \|B\mathbf{r}_0|_{\mathcal{R}(B)}\|_2. \quad \blacksquare$$

Preconditioned CGLS

$$C = (\tilde{L}\tilde{L}^\top)^{-1} \in \mathbf{R}^{m \times m}, SPD$$

Precondition

$$AA^\top \mathbf{y} = \mathbf{b}$$

as

$$A'\mathbf{y}' = \mathbf{b}' \quad (**)$$

where

$$A' = \tilde{L}^{-1}AA^\top\tilde{L}^{-\top},$$

$$\mathbf{y}' = \tilde{L}^\top \mathbf{y},$$

$$\mathbf{b}' = \tilde{L}^{-1}\mathbf{b}.$$

Since

$$\tilde{L}A'\tilde{L}^{-1} = AA^\top C = AB,$$

$$\lambda_i(A') = \lambda_i(AB) = \sigma_i^2, \quad i = 1, \dots, m.$$

Theorem 23 *The residual $\mathbf{r} = \mathbf{b} - AA^T\mathbf{y}$ of the k -th step of preconditioned CGLS (CG applied to (**)) satisfies*

$$\|\mathbf{r}_k\|_{(AA^T)^{-1}} = \|e_m\|_{AA^T} \leq 2 \left(\frac{\sigma_1 - \sigma_m}{\sigma_1 + \sigma_m} \right)^k \|\mathbf{r}_0\|_{(AA^T)^{-1}}. \quad \blacksquare$$

Similar convergence behaviours expected for
AB-GMRES, BA-GMRES,
and preconditioned CGLS methods,
using the same preconditioner C .

Choice of B

Besides satisfying

$$\mathcal{R}(A) = \mathcal{R}(B^\top) \text{ and } \mathcal{R}(A^\top) = \mathcal{R}(B),$$

B should satisfy $AB \approx I_m$ or $BA \approx I_n$.

Simple choice:

$$B = CA^\top, C = \{\text{diag}(A^\top A)\}^{-1}$$

when $m \geq n = \text{rank}A$,

$$B = A^\top C, C := \{\text{diag}(AA^\top)\}^{-1}$$

when $\text{rank}A = m \leq n$.

**Application of
Robust Incomplete Factorization (RIF)**
(Benzi and Tuma, '03)

$$A^T A \approx LDL^T,$$

$$A^T A \approx Z^{-T} D Z^{-1},$$

where $A \in \mathbf{R}^{m \times n}$ with $m \geq n = \text{rank} A$,

Z : upper triangular matrix,

L : lower triangular matrix.

Use of (incomplete) $A^T A$ -orthogonalization.

Low memory requirement.

RIF Method

Let $Z = F = [e_1, e_2, \dots, e_n]$

For $j = 1, \dots, n$ Do

 Compute $u_j = Az_j$

 Compute $d_j = (u_j, u_j)$

 For $i = j + 1, \dots, n$ Do:

 Compute $v_i = Ae_i$

 Compute $\theta_{ij} = \frac{(v_i, u_j)}{d_j}$

 IF $\theta_{ij} > \tau$

 Store $L(i, j) = \theta_{ij}$

 ENDIF

 Compute $z_i = z_i - \theta_{ij}z_j$

 Drop the elements in z_i smaller than τ

 EndDo

EndDo

Numerical experiments

PC: Dell Precision 690

CPU: 3.00 GHz, Memory: 16 GB

Program, compiler: GNU C/C++ 3.4.3

Linear least squares problems

$$\min_{\mathbf{x} \in \mathbf{R}^n} \|\mathbf{b} - A\mathbf{x}\|_2, \quad A \in \mathbf{R}^{m \times n}$$

1. Over-determined case ($m \geq n$)

Test matrices A :

- Generated by MATLAB command “sprandn” .
- Specified density and condition number.
- Value of nonzero elements:
 random (normal distribution)
- Pattern of nonzero elements: random.

\mathbf{b} : also random, inconsistent ($\mathbf{b} \notin \mathcal{R}(A)$).

Convergence judged by $\frac{\|A^T \mathbf{r}\|_2}{\|A^T \mathbf{b}\|_2}$, $\mathbf{r} = \mathbf{b} - A\mathbf{x}$.

$\mathbf{x}_0 = \mathbf{0}$.

Test matrices (L)

$$m = 30,000, n = 3,000$$

density: 0.1%

Name	Condition number
RANDL1	1.9×10
RANDL2	1.6×10^2
RANDL3	1.3×10^3
RANDL4	2.0×10^4
RANDL5	1.3×10^5
RANDL6	1.3×10^6
RANDL7	1.3×10^7

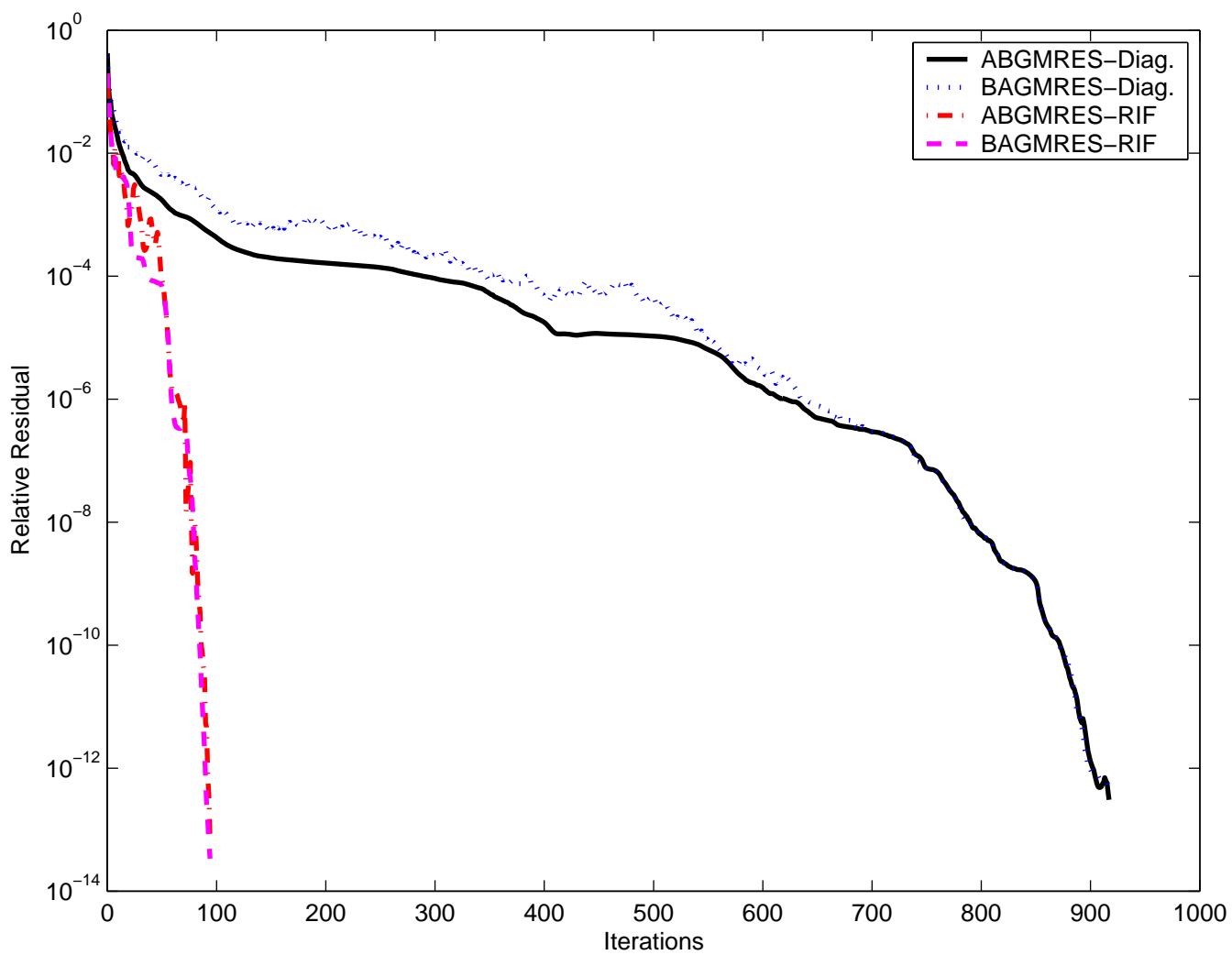
Fig. 1

Comparison of full AB-GMRES and BA-GMRES

with diagonal-scaling
and RIF preconditioner ($\tau = 0.8$)

(RANDL3)

($\|A^T \mathbf{r}\|_2 / \|A^T \mathbf{b}\|_2$ vs. iterations)



The effect of the restart period k
in the BA-GMRES(k)-RIF method
(over-determined problem).

RANDL5 ($\tau = 0.8$)	k	100	140	180	220	260	≥ 295
	iter	755	668	587	498	453	295
	time	25.05	24.81	24.14	22.62	22.15	*14.27
RANDL6 ($\tau = 0.07$)	k	160	200	240	280	300	≥ 318
	iter	2,470	2,085	1,856	1,311	599	318
	time	144.68	130.08	121.72	92.88	48.92	*26.73
RANDL7 ($\tau = 0.02$)	k	200	280	320	340	360	≥ 362
	iter	2,594	2,168	1,567	900	506	362
	time	179.83	165.79	129.07	80.13	50.99	*37.26

k : restart period, iter: number of iterations

time: computation time (sec.)

Convergence criterion: $\|A^T \mathbf{r}\|_2 / \|A^T \mathbf{b}\|_2 < 10^{-6}$.

The effect of the RIF parameter τ
for problem RANDL3.

	τ	0.9	0.8	0.7	0.6	0.5	0
CGLS-RIF	iter	83	72	77	65	67	1
	time	5.39	*5.38	5.42	5.43	5.59	68.00
LSQR-RIF	iter	83	73	78	66	68	1
	time	5.39	*5.38	5.42	5.43	5.60	68.00
RCGLS-RIF	iter	79	70	73	64	66	1
	time	5.99	5.86	5.96	5.85	6.08	67.99
BA-GMRES-RIF	iter	70	60	73	64	66	1
	time	5.54	5.47	5.64	5.59	5.63	67.99

iter: number of iterations

time: computation time (sec.)

Convergence criterion: $\|A^T \mathbf{r}\|_2 / \|A^T \mathbf{b}\|_2 < 10^{-6}$.

The effect of the RIF parameter τ
for problem RANDL6.

	τ	0.09	0.08	0.07	0.06	0.05	0
CGLS-RIF	iter	670	674	615	706	658	1
	time	34.38	35.39	33.67	38.17	37.31	60.00
LSQR-RIF	iter	680	685	645	736	701	1
	time	34.87	35.50	34.15	37.21	37.41	60.00
RCGLS-RIF	iter	333	324	317	313	307	1
	time	34.11	33.54	33.22	33.39	33.48	60.01
BA-GMRES-RIF	iter	335	325	318	315	309	1
	time	27.03	26.77	*26.73	27.16	27.45	60.01

iter: number of iterations

time: computation time (sec.)

Convergence criterion: $\|A^T \mathbf{r}\|_2 / \|A^T \mathbf{b}\|_2 < 10^{-6}$.

Comparison of convergence

$\|A^T \mathbf{r}\|_2 / \|A^T \mathbf{b}\|_2$ vs. number of iterations

Fig.2: Diagonal scaling (RANDL5)

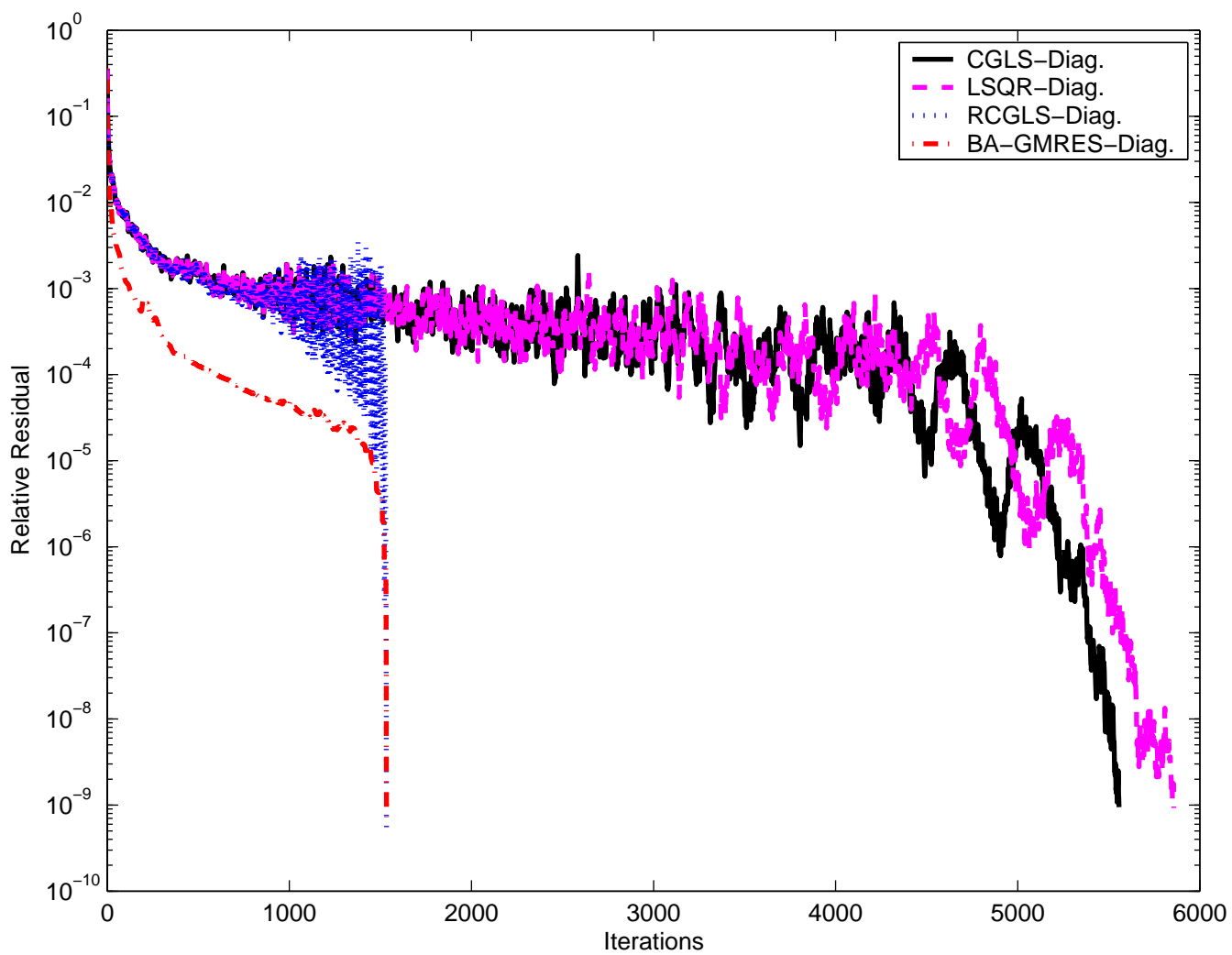


Fig.3: RIF (RANDL5)

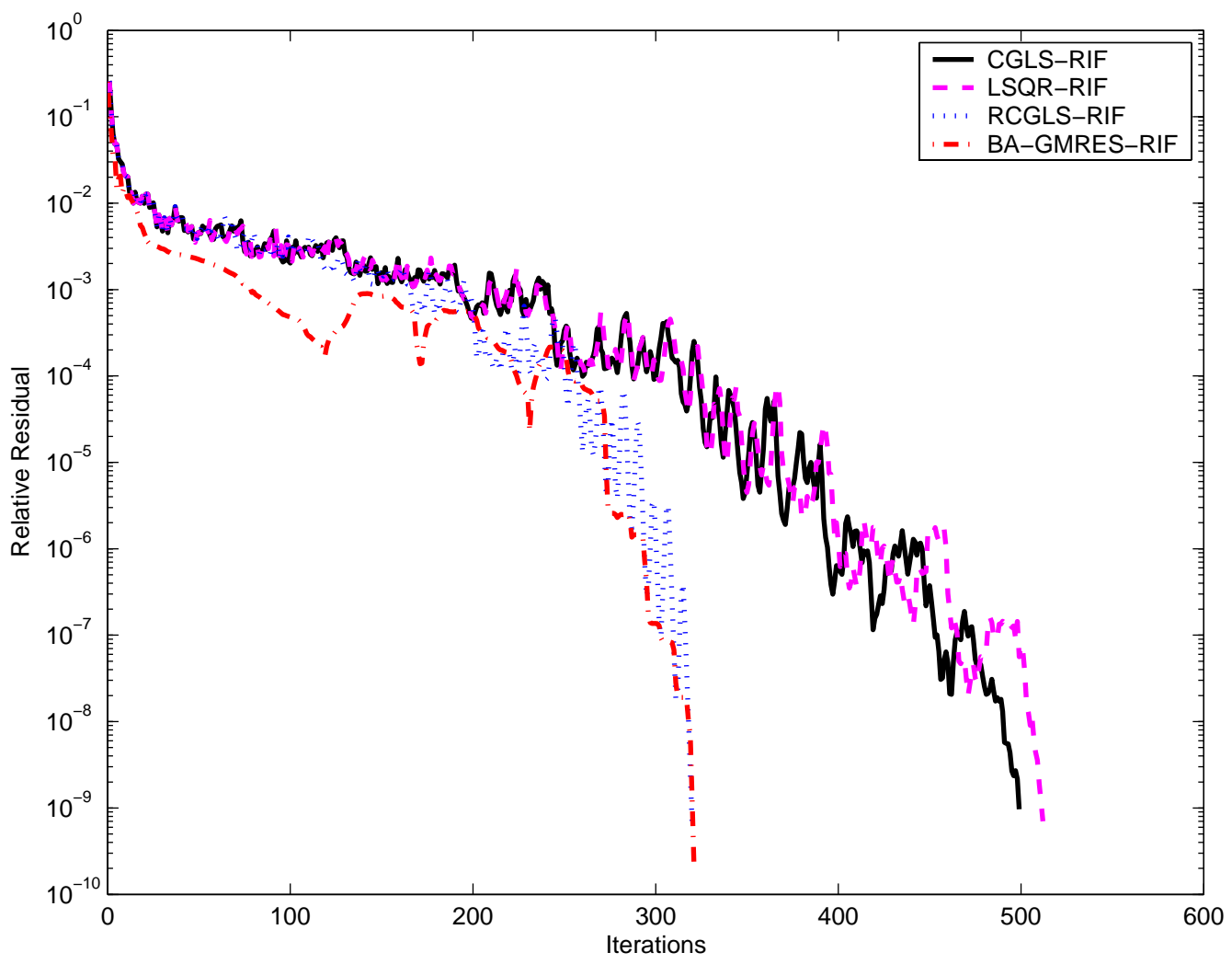


Fig.4: Diagonal scaling (RANDL6)

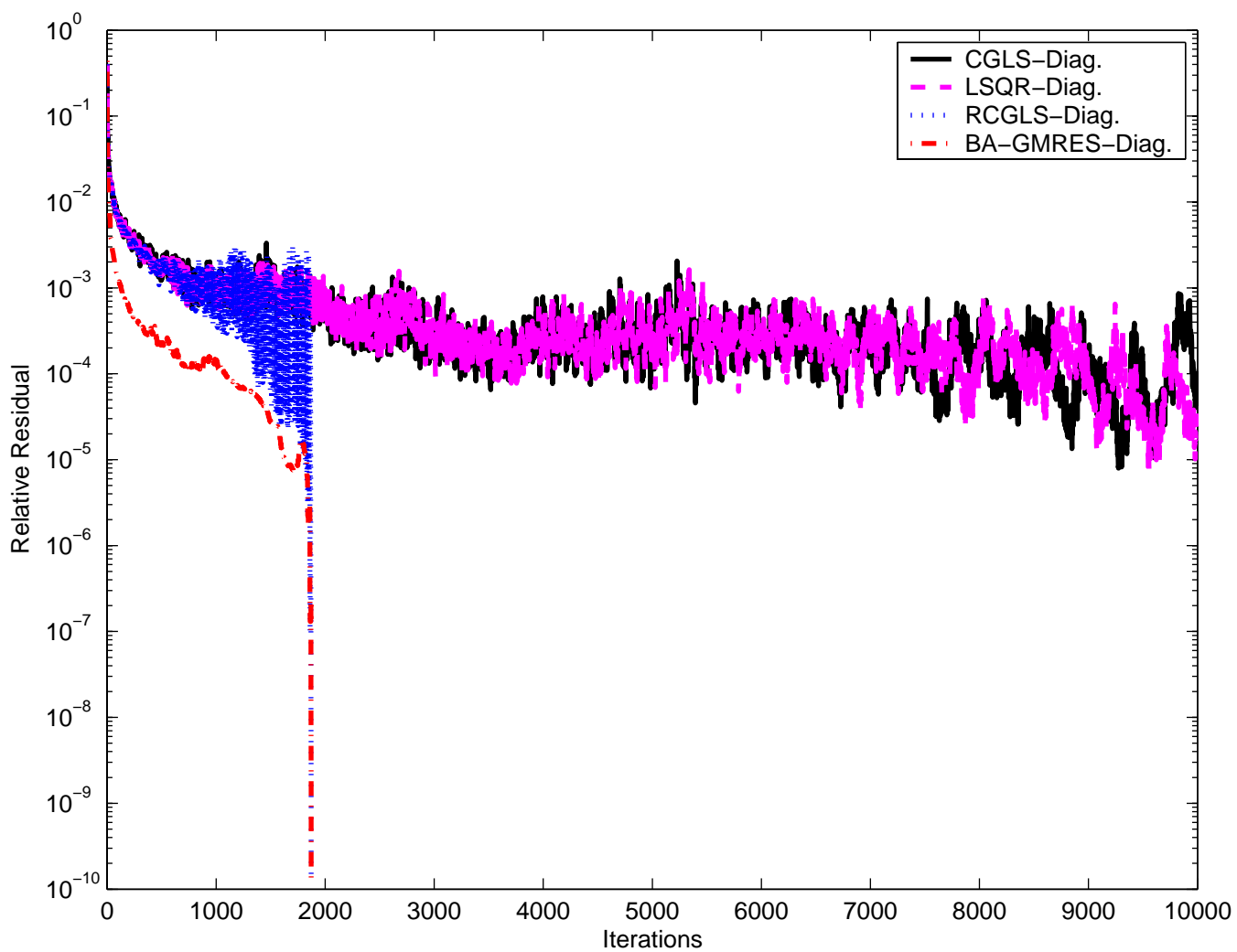
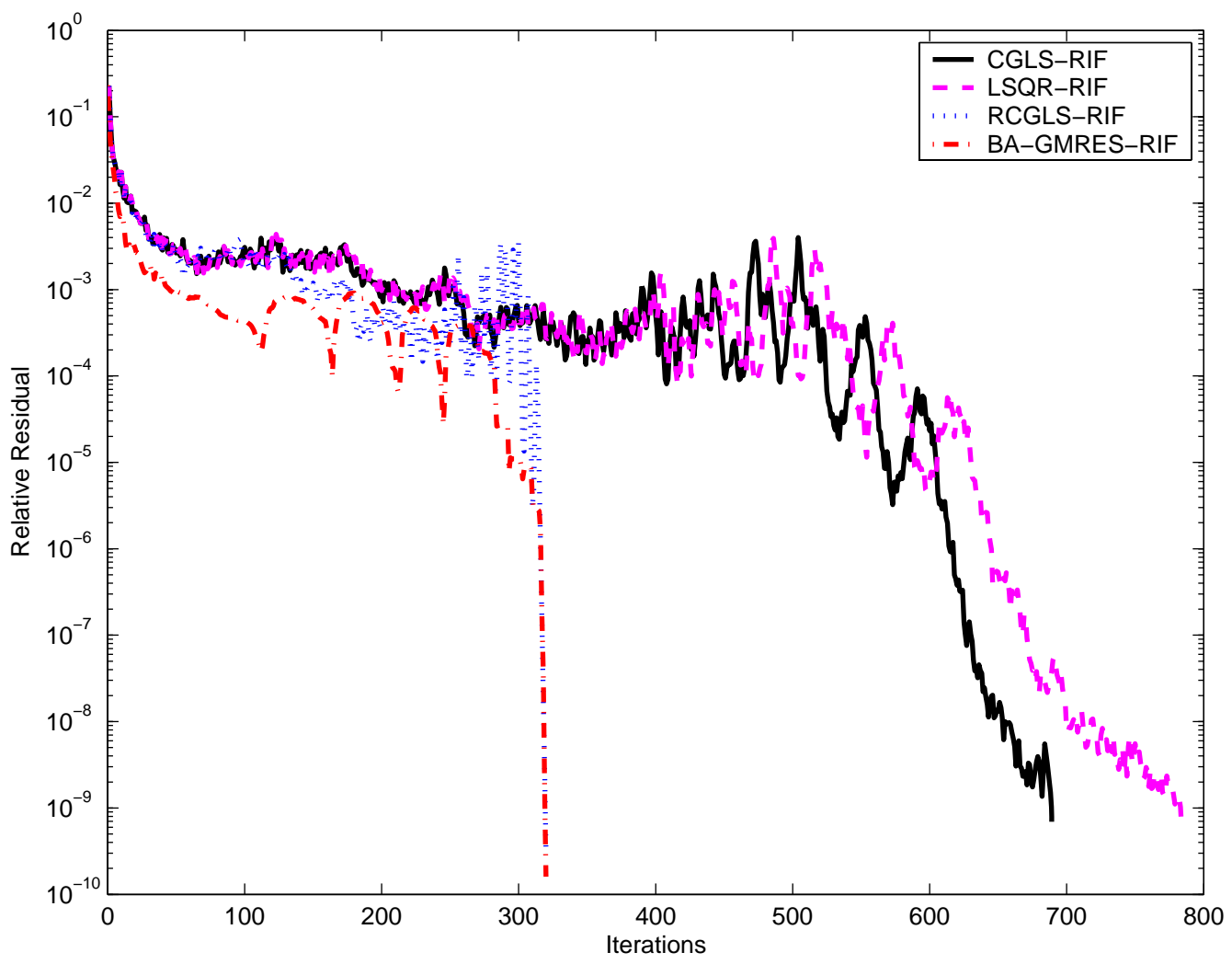


Fig.5: RIF (RANDL6)



Comparison of CPU time

	CGLS		LSQR		RCGLS		BA-GMRES	
	-diag.	-RIF	-diag.	-RIF	-diag.	-RIF	-diag.	-RIF
RANDL1 ($\tau = 0.5$)	35 *0.10	14 4.98	35 *0.10	14 4.98	35 0.16	14 4.99	35 0.14	14 4.99
RANDL2 ($\tau = 0.7$)	214 *0.61	21 5.10	214 *0.61	21 5.10	208 2.77	21 5.13	193 2.28	21 5.11
RANDL3 ($\tau = 0.8$)	742 2.08	72 5.38	740 *2.07	73 5.38	697 26.30	70 5.62	622 20.70	60 5.47
RANDL4 ($\tau = 0.5$)	1,147 *3.22	85 6.38	1,154 3.38	85 6.38	1,062 59.35	84 7.17	1,069 59.41	82 6.62
RANDL5 ($\tau = 0.9$)	4,897 13.74	470 *12.78	5,064 14.03	401 11.79	1,521 119.70	305 14.42	1,522 118.87	299 13.91
RANDL6 ($\tau = 0.07$)	10,551 29.65	615 33.67	11,088 30.21	645 34.15	1,861 177.94	317 26.93	1,862 176.93	318 *26.73
RANDL7 ($\tau = 0.02$)	32,143 89.93	1,951 102.28	35,034 91.31	2,443 128.40	1,914 195.63	371 40.07	1,899 183.90	362 *37.26

First row: number of iterations

Second row: computation time (seconds).

Convergence criterion: $\|A^T r\|_2 / \|A^T b\|_2 < 10^{-6}$.

Problems from animal breeding studies
and meteorology (HIRLAM)

Name	m	n	nnz	density
SMALL	3,140	1,988	8,510	1.4%
MEDIUM	9,397	6,119	25,013	0.04%
LARGE	28,524	17,264	75,018	0.02%
VLARGE	174,193	105,882	463,303	0.003%
HIRLAM	1,385,270	452,200	2,718,200	0.0004%

	CGLS		LSQR		BAGMRES	
	-diag.	-RIF	-diag.	-RIF	-diag.	-RIF
SMALL ($\tau = 0.2$)	125 *0.06	59 0.33	125 *0.06	59 0.33	124 0.54	58 0.49
MEDIUM ($\tau = 0.3$)	128 *0.20	64 2.10	128 *0.20	64 2.10	123 1.67	62 2.45
LARGE ($\tau = 0.5$)	133 *0.67	73 15.83	133 *0.67	73 15.83	131 5.81	71 17.93
VLARGE ($\tau = 0.8$)	171 6.00	137 36.56	170 *5.97	137 36.57	166 58.45	136 73.45
HIRLAM ($\tau = 0.9$)	180 *48.16	164 204.44	180 48.20	164 204.46	170 294.05	163 464.93

First row: number of iterations,

Second row: computation time (seconds).

Convergence criterion: $\|A^T \mathbf{r}\|_2 / \|A^T \mathbf{b}\|_2 < 10^{-6}$.

Explanation for better convergence of GMRES:

Modified Gram-Schmidt process in GMRES
(explicit orthogonalization):
Robust against rounding error
esp. for ill-conditioned case

vs.

three-term recurrence in CG
(implicit orthogonalization)

2. Under-determined case ($m < n$)

$$\min_{\mathbf{x} \in \mathbf{R}^n} \|\mathbf{b} - A\mathbf{x}\|_2, \quad A \in \mathbf{R}^{m \times n} \quad (m < n).$$

Minimum norm least squares (pseudo-inverse)
solution:

$$AA^T \mathbf{y} = \mathbf{b}, \quad \mathbf{x} = A\mathbf{y}$$

Previous approach:

Apply (preconditioned) CG: CGNE

Test random matrices

RANDLnT: 3,000 × 30,000, density: 1.5%
(transpose of RANDLn).

$$\mathbf{b} = A\mathbf{x}^* \text{ where } \mathbf{x}^* = (1, \dots, 1)^T.$$

Convergence judged by $\|\mathbf{r}\|_2 / \|\mathbf{b}\|_2$
(rank $A = m$: consistent system)

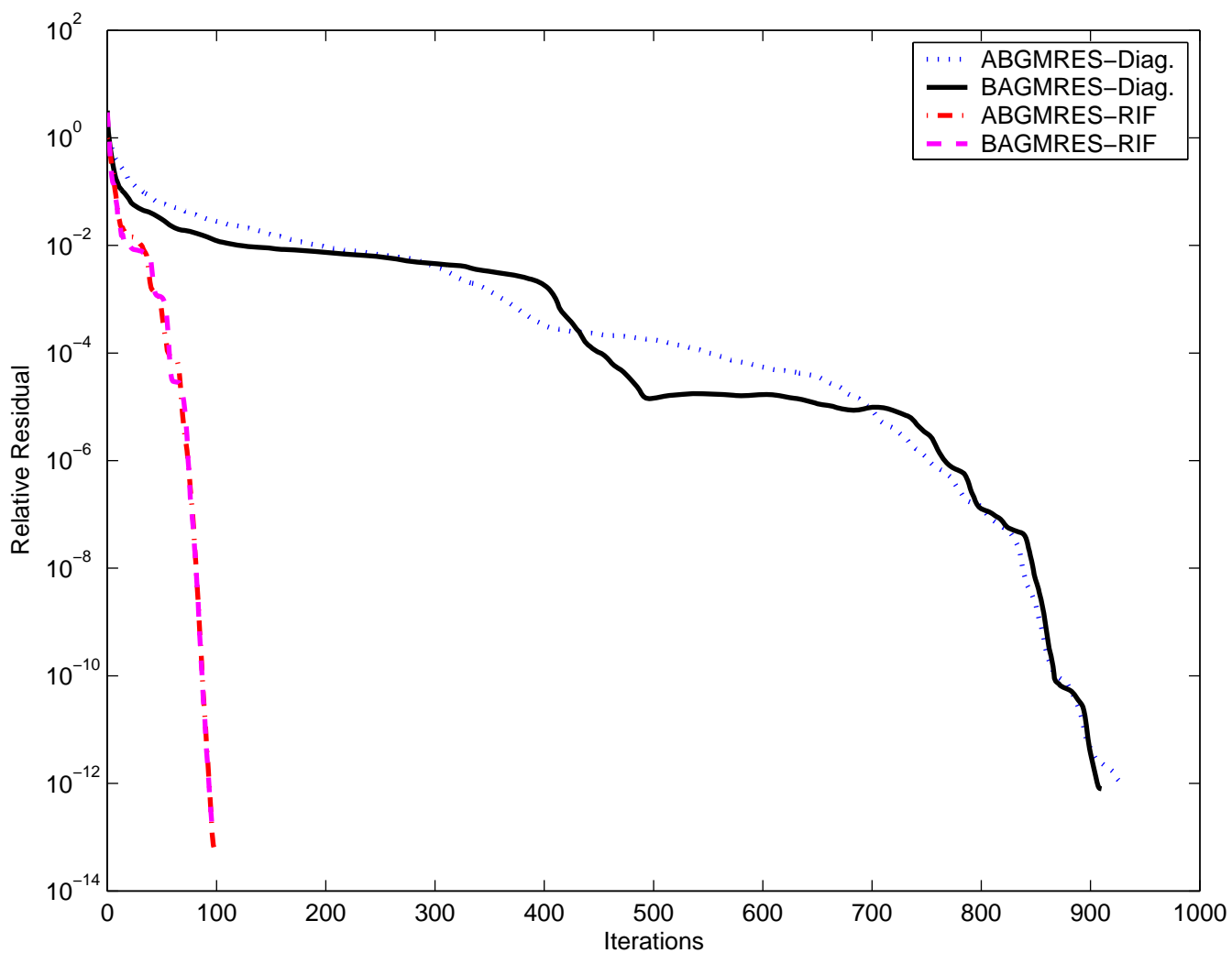
Fig. 6

Comparison of full AB-GMRES and BA-GMRES

with diagonal-scaling
and RIF preconditioner

(RANDL3T)

($\|\mathbf{r}\|_2/\|\mathbf{b}\|_2$ vs. iterations)



Comparison of convergence

$\|r\|_2/\|b\|_2$ vs. number of iterations

Fig.7: Diagonal scaling (RANDL5T)

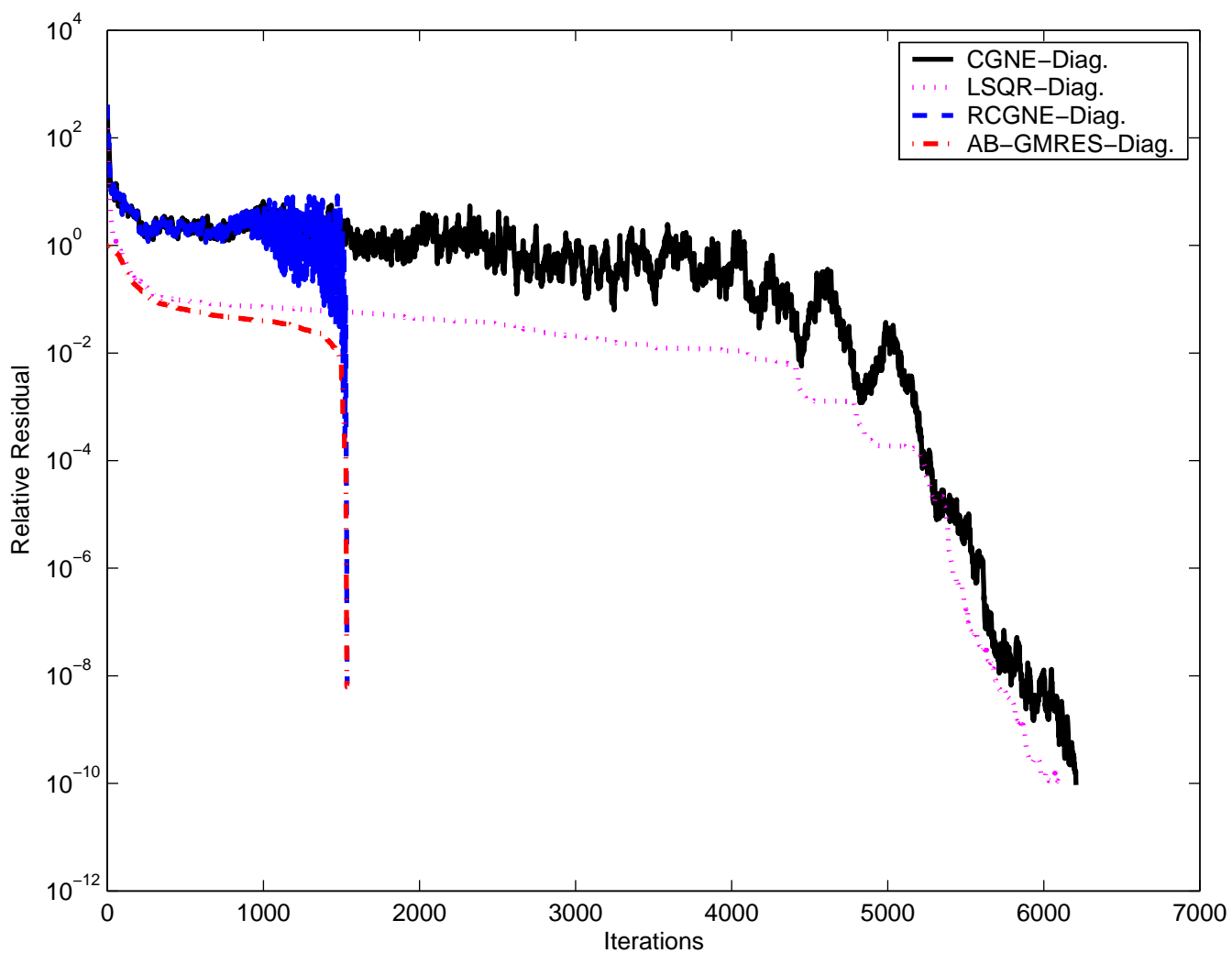


Fig.8: RIF (RANDL5T)

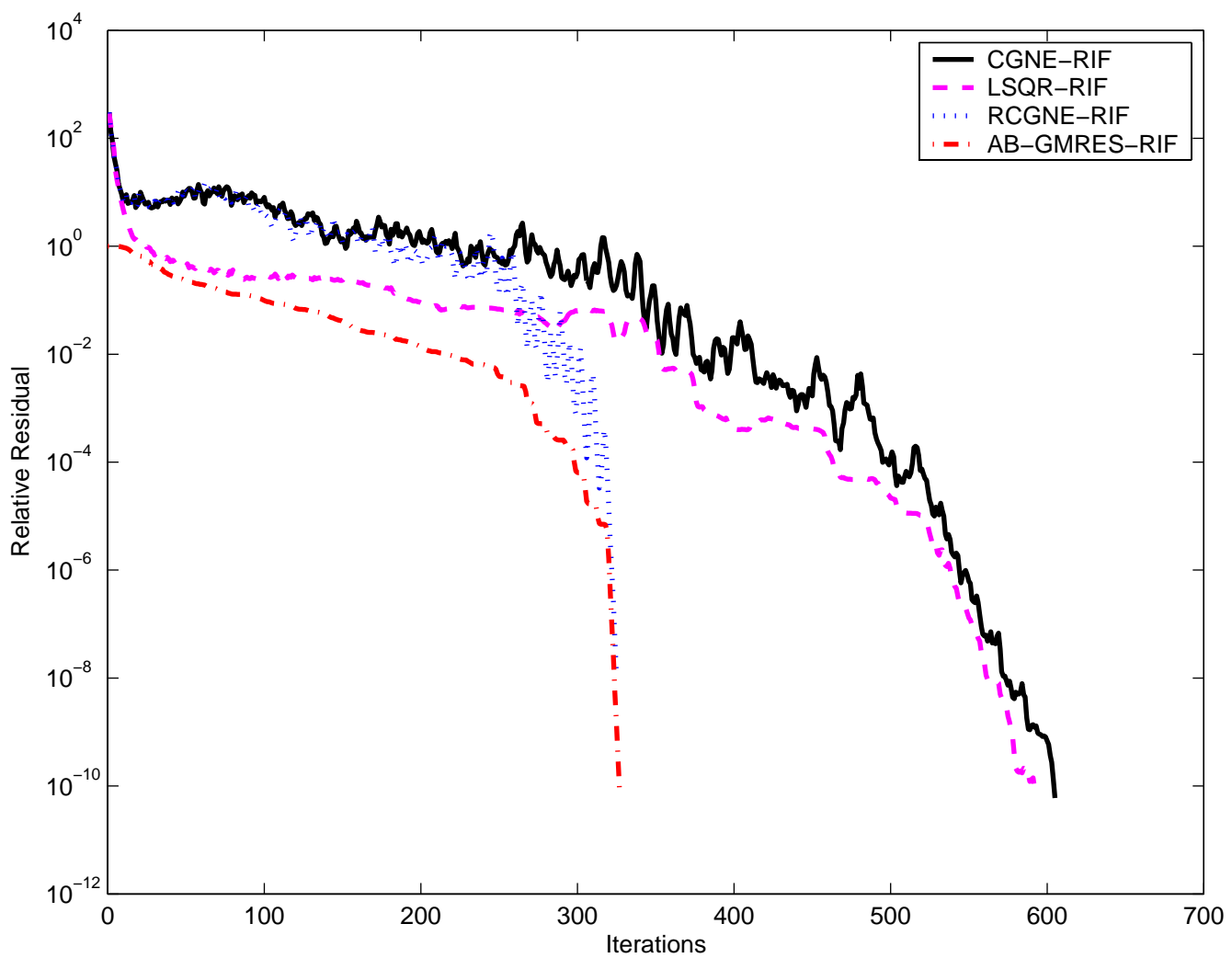


Fig.9: Diagonal scaling (RANDL6T)

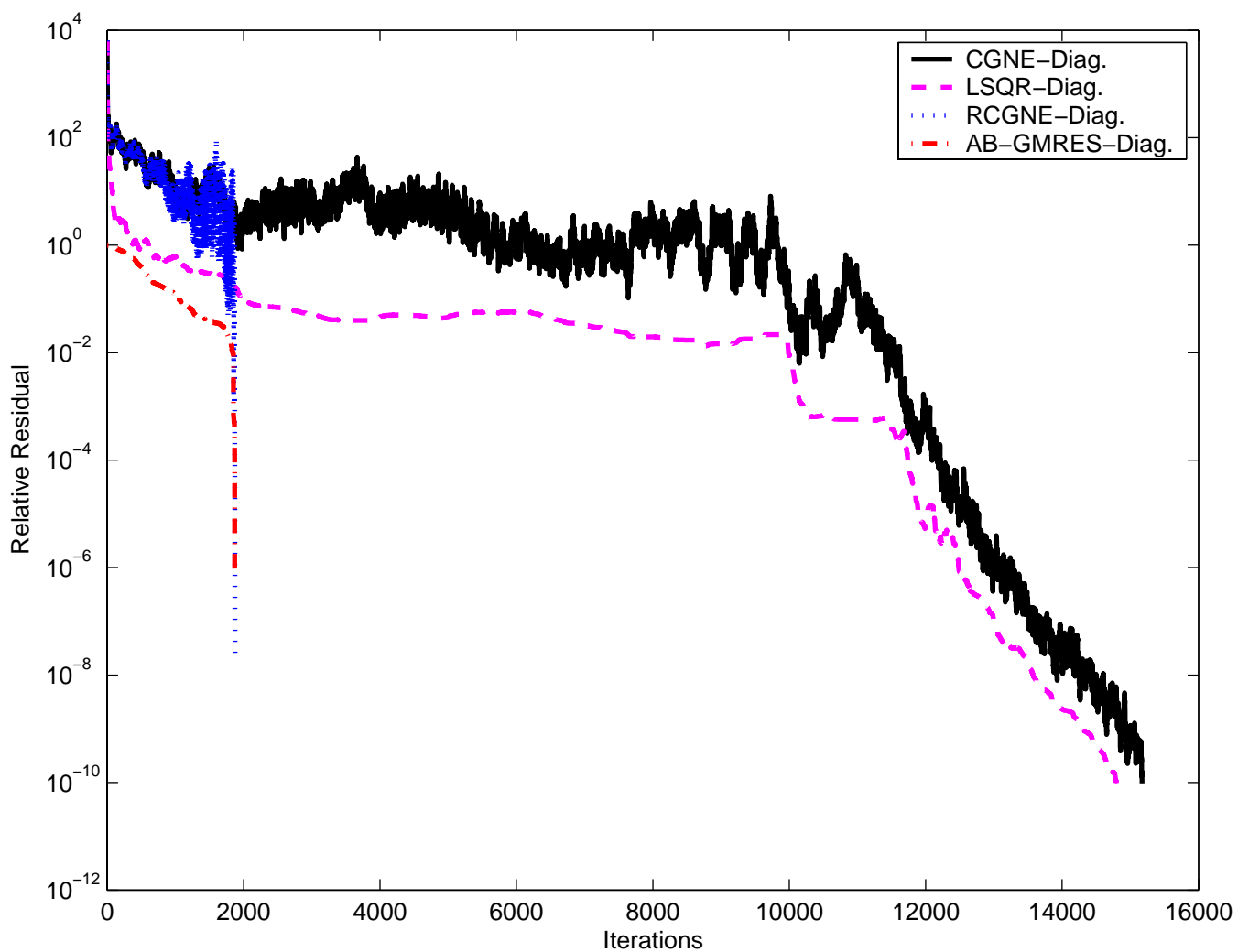
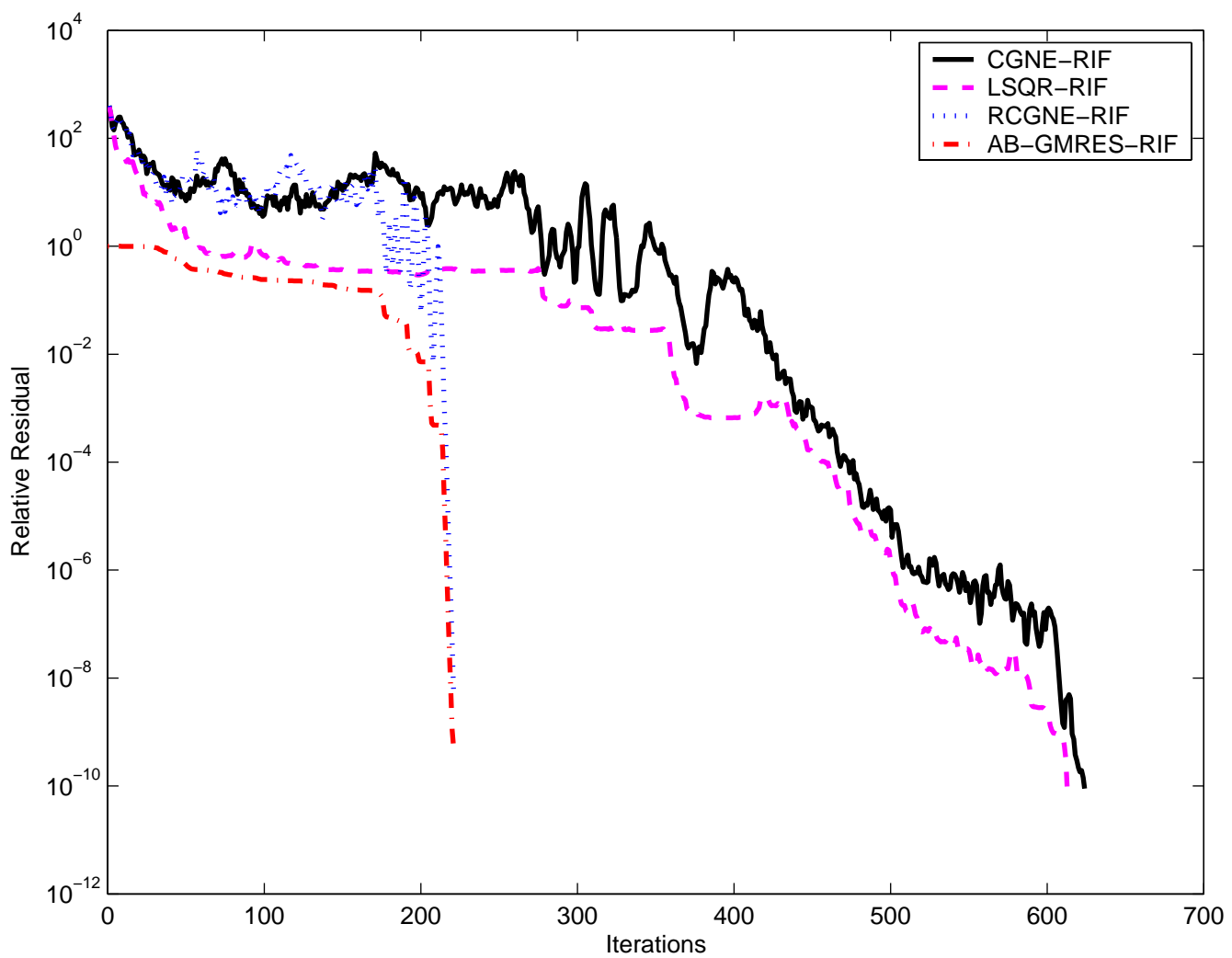


Fig.10: RIF (RANDL6T)



Comparison of CPU time

	CGNE		LSQR		RCGNE		AB-GMRES	
	-diag.	-RIF	-diag.	-RIF	-diag.	-RIF	-diag.	-RIF
RANDL1T ($\tau = 0.4$)	37 *0.15	12 5.01	37 *0.15	12 5.02	37 0.23	12 5.02	37 0.17	12 5.01
RANDL2T ($\tau = 0.7$)	259 *1.06	25 5.16	256 *1.06	25 5.16	252 4.22	25 5.17	247 3.75	25 5.17
RANDL3T ($\tau = 0.8$)	838 *3.43	81 5.53	823 *3.43	80 5.53	783 33.87	77 5.81	754 30.56	75 5.67
RANDL4T ($\tau = 0.5$)	1,464 5.97	116 6.94	1,407 *5.96	114 6.94	1,223 79.67	106 7.45	1,187 73.67	106 7.21
RANDL5T ($\tau = 0.9$)	5,548 22.61	544 13.88	5,414 22.71	539 *13.86	1,535 123.80	322 15.58	1,533 121.58	322 15.11
RANDL6T ($\tau = 0.01$)	12,837 52.38	514 39.04	12,486 50.10	502 38.99	1,873 182.51	219 27.43	1,871 179.85	218 *26.99
RANDL7T ($\tau = 0.04$)	38,397 156.01	3,078 94.19	37,792 152.07	2,979 91.69	2,240 366.88	451 44.49	2,238 353.92	450 *43.76

First row: number of iterations

Second row: computation time (seconds).

Convergence criterion: $\|r\|_2/\|b\|_2 < 10^{-6}$.

Memory requirements

Intermediate memory required for each method for k iterations.

	$\dim(m)$	$\dim(n)$	$\dim(k)$	total
CGLS	r, Ap	$x, p, A^T r$		$2m + 3n$
CGNE	r, Ap	$x, p, A^T r$		$2m + 3n$
LSQR	u	v, w, x		$m + 3n$
AB-GMRES(k)	V, w	x	y, e	$(k + 1)m + n + 2k + k^2/2$
BA-GMRES(k)		V, w, x	y, e	$(k + 2)n + 2k + k^2/2$

Conclusions

Proposed two methods
for least squares problems
using GMRES on

1. $\min_{\mathbf{z} \in \mathbf{R}^m} \|\mathbf{b} - AB\mathbf{z}\|_2,$
2. $\min_{\mathbf{x} \in \mathbf{R}^n} \|B\mathbf{b} - BA\mathbf{x}\|_2.$

Sufficient conditions for B :

$$\mathcal{R}(B) = \mathcal{R}(A^\top), \quad \mathcal{R}(B^\top) = \mathcal{R}(A).$$

Convergence analysis.

Numerical experiments:

GMRES faster than CGLS type methods
when used with RIF
for ill-conditioned problems.

Thank you!

Preprint:

<http://research.nii.ac.jp/TechReports/07-009E.pdf>