GMRES Methods for Tomographic Reconstruction with an Unmatched Back Projector

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Joint work with Ken Hayami and Keiichi Morikuni funded by JSPS



X-Ray Computed Tomography (CT)





Lab scanner

Medical scanner



Synchrotron SPring-8





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X-Ray CT and the Radon Transform

The Principle

Send X-rays through the object f at many angles, and measure the attenuation g.



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f = 2D object/image



$$g = \mathcal{R} f = \text{Radon transform of } f$$
$$= \text{sinogram}$$



This Work Focuses on Unmatched Projectors

My interest in this topic arose when we started writing a *new book* on computational algorithms for computed tomography – in particular when write the chapters on algebraic iterative reconstruction methods.



X-Ray CT – Forward and Back Projections

Forward projection \mathcal{R} , the Radon transform *models the scanner physics*. Back projection \mathcal{B} = adjoint(\mathcal{R}) is a *mathematical abstraction*.

> Multiplication with $A \leftrightarrow action$ of forward projector \mathcal{R} . Multiplication with $B \leftrightarrow action$ of back projector \mathcal{B} .

When we can store A then we use A^T for back projection, and our iterative methods solve (weighted) normal equations $A^T A x = A^T b$.

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When A is too large to store, we must use matrix-free multiplications of the forward projector and back projector.

HPC software: computational efficiency takes priority $\rightarrow B \neq A^T$.

We are now faced with the unmatched normal equations

BAx = Bb.

The matrix BA usually has some eigenvalues with negative real part, so we cannot use stationary iterative methods with A^T replaced by B.

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"Fix" a Stationary Iterative Method

Unmatched pair from *ASTRA* software package, image has 64×64 pixels, 90 proj. angles, 60 detector elements, no noise, min $\Re \lambda_i = -6.4 \cdot 10^{-8}$.



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Define the Shifted BA Iteration (T. Elfving)

$$x^{k+1} = (1 - \alpha \omega) x_k + \omega \mathbf{B} (b - \mathbf{A} x_k), \qquad \omega > 0$$

Convergence condition:

$$\Re (\texttt{eig}({m B}{m A})) + lpha > {m 0}$$
 .

Just choose α large enough that this is satisfied.

Drawback: in addition to relax. param. ω we must also choose shift α .

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Alternative: Solve the Unmatched Normal Equations

Instead of "fixing" an algorithm designed for solving another problem, just solve the unmatched normal equations in one of the forms

$$\boxed{BAx = Bb} \quad \text{or} \quad \boxed{ABy = b}, \quad x = By$$

The left- or right-preconditioned GMRES method for (A, b) immediately presents itself as a good choice with B as the preconditioner.

<u>BA-GMRES</u> solves BAx = Bb with B as a left preconditioner.

<u>AB-GMRES</u> solves A B y = b, x = B y with B as a right preconditioner.

Advantages:

- these methods always converge,
- no need for relaxation parameter or shift parameter.

Perturbation theory: Elfving, H (2018) and H, Hayami, Morikuni (subm.).

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Solving the Unmatched Normal Equations

Hayami, Yin, Ito (2010)

<u>AB-GMRES</u> solves min_y $||ABy - b||_2$, x = By (B = right precond.)

 $\triangleright \min_{x} ||Ax - b||_{2} = \min_{z} ||ABz - b||_{2} \text{ holds for all } b \text{ if an only} \\ \text{if } \operatorname{range}(AB) = \operatorname{range}(A), \text{ e.g., if } \operatorname{range}(B) = \operatorname{range}(A^{T}).$

<u>BA-GMRES</u> solves $\min_{x} \|BAx - Bb\|_{2}$ (B = left preconditioner)

▷ the problems $\min_{x} ||Ax - b||_2$ and $\min_{x} ||BAx - Bb||_2$ are equivalent for all *b* if and only if $\operatorname{range}(B^TBA) = \operatorname{range}(A)$, e.g., if $\operatorname{range}(B^T) = \operatorname{range}(A)$.

Both methods use the same Krylov subspace $\mathcal{K}_k(BA, Bb)$ for the solution, but they use different objective functions.

Conditions are difficult/impossible to check in a given X-ray CT problem

 \ldots but it works \hookrightarrow

Relation to LSQR and LSMR with a Matched Transpose

H, Hayami, Morikuni (submitted)

AB-GMRES with $B = A^T$ computes $x_k = A^T u_k$ with $u_k = \arg \min_{u \in \mathcal{K}_k(AA^T, b)} ||b - AA^T u||_2^2$. Let $r_k = b - Ax_k$; the method minimizes

$$\|r_k\|_2^2 = \|r_k|_{\mathsf{range}(A)}\|_2^2 + \mathsf{constant}$$

and so does LSQR; they produce the same iterates (in ∞ precision).

BA-GMRES with $B = A^T$ applies GMRES to

$$A^T A x = A^T b \qquad \longleftrightarrow \qquad \min_{x} \|b - A x\|_2.$$

Equivalent to applying MINRES to the normal equations $A^T A x = A^T b$ which, in turn, is equivalent to **LSMR** (in ∞ precision).

Reconstr. Error, Noisy Data, Matrix is $252\,000 \times 176\,400$

Image has 420 \times 420 pixels, 600 projection angles, 420 detector pixels.



- Semi-convergence (see next slide \hookrightarrow) is evident for both methods.
- Same minimum reconstruction error $||x_k \bar{x}||_2 / ||\bar{x}||_2 \approx 0.10$ for both.
- Slightly fewer iterations for AB-GMRES in this example.

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Analysis of Semi-Convergence: Split the Error

Let \bar{x}_k denote the iterates for a noise-free right-hand side. We consider:



The iteration error decreases, and we expect the noise error to increase.

Then we have *semi-convergence*, when the noise error starts to dominate:



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Semi-Convergence of GMRES

Some insight has been obtained.

- Calvetti, Lewis, Reichel (2002): if the noise-free data lies in a finite-dimensional Krylov subspace, and if GMRES is equipped with a suitable stopping rule, then the GMRES-solution converges to the exact solution \bar{x} as the noise goes to zero.
- Gazzola, Novati (2016): if Ax = b satisfies the discrete Picard condition (DPC) and if the left singular vectors of the Hessenberg matrices of two consecutive GMRES steps resemble each other – then the Hessenberg systems in GMRES also satisfy the DPC.

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Our lesson: if all SVD components corresponding to the large singular values are captured in order of decreasing magnitude when GMRES is applied to Ax = b, then GMRES will exhibit semi-convergence.

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A complete understanding of these aspects has not emerged yet. Here we rely on insight from numerical experiments.

BA-GMRES: SVD Analysis, Small Matrix 23040 \times 16384



- Left plot is typical for X-ray CT problems; no rank deficiency.
- As k increases we capture more SVD components in x_k .
- At k = 30 we already capture the first 11000 exact SVD components.
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BA-GMRES: SVD Analysis - Now With Noisy Data



- Left plot is typical for X-ray CT problems; no rank deficiency.
- As k increases we capture more SVD components in x_k .
- At k = 30 we already capture the first 11000 exact SVD components.
- Eventually we include noisy SVD components = semi-convergence.
- We obtain the best reconstruction after $k \approx 50$ iterations.

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GMRES and Unmatched Projectors

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BA-GMRES: SVD Analysis – With More Noise



- Left plot: the "noise floor" increases..
- As k increases we capture more SVD components in x_k .
- At k = 30 we already capture the first 11000 exact SVD components.
- Eventually we include noisy SVD components = semi-convergence.
- Now we obtain the best reconstruction after $k \approx 20$ iterations.

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Stopping Rules

We must terminate the iterations at the point of semi-convergence.

• Discrepancy principle (DP): terminates the iterations as soon as the residual norm is smaller than the noise level:

 k_{DP} = the smallest k for which $||b - Ax_k||_2 \le \tau ||e||_2$

where $\tau \ge 1 =$ safety factor when we have a rough estimate of $||e||_2$.

• NCP criterion: uses the normalized cumulative periodogram to perform a spectral analysis of the residual vector $\overline{b} - A x_k$ and identifies when the residual is close to being white noise – which indicates that all available information has been extracted from the noisy data.

For those who are curious: the L-curve criterion does not work, and we cannot implement generalized cross validation (GCV) efficiently.

Stopping Rules: Tests With 2 Different Back Projectors



Both DP and NCP stop a bit too early – better than stopping too late.

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Conclusion

Facts

- Unmatched projector pairs in X-ray CT are here to stay.
- Need efficient iterative reconstruction methods for unmatched pairs.

Different approaches

- Use a classical method that ignores the mismatch \rightarrow hope for the best.
- Modify a classical method, e.g., as in the Shifted BA Iteration
 → but this requires an estimate of the leftmost eigenvalue.
- Use a method that solves the unmatched normal equations \rightarrow AB-GMRES and BA-GMRES are the choices here.

Our contribution

- The AB- and BA-GMRES methods exhibit semi-convergence.
- They are suited as iterative regularization methods in X-ray CT.
- We have stopping rules that work well.
- Next step: flexible preconditioning to enforce nonnegativity.