AB– and BA–GMRES Methods for X-Ray CT with an Unmatched Back Projector

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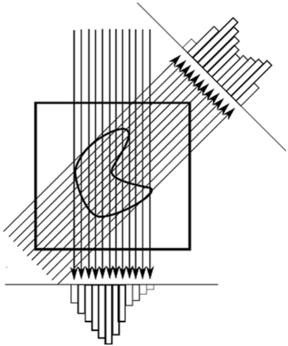
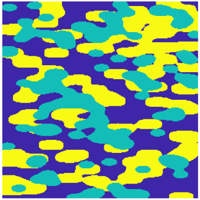
Prologue: X-Ray CT in 2D – and the Radon Transform

The Principle

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

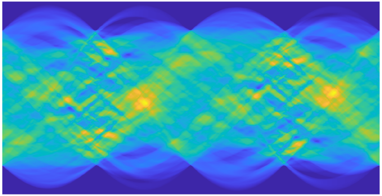


f = 2D object/image



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

= sinogram



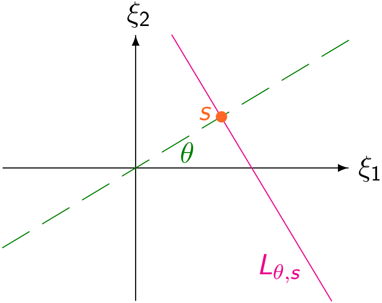
Prologue: Forward and Back Projections

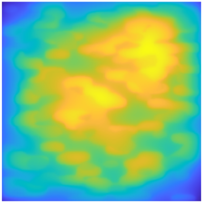
Forward projection $\mathcal{R}$, the Radon transform models the scanner physics via integration of the function f along lines $L_{\theta,s}$

$$\mathcal{R}[f](\theta,s) = \int_{L_{\theta,s}} f(\xi_1,\xi_2)\, d\ell = g(\theta,s) = \text{sinogram} \ .$$

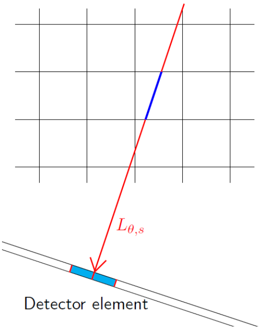
Back projection $\mathcal{B} = \text{adjoint}(\mathcal{R})$, an abstraction, smears g back along $L_{\theta,s}$

$$\mathcal{B}[g](\xi_1,\xi_2) = \int_0^{2\pi} g(\theta, \xi_1 \cos\theta + \xi_2 \sin\theta)\, d\theta \ .$$



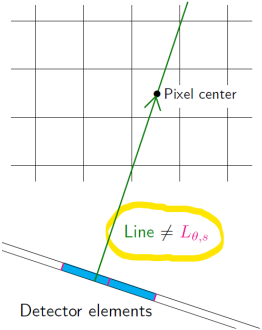


Ray/Pixel Driven Discretization Models



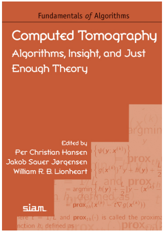
Forward line model

Ray driven



Back projection model

Pixel driven



Details here

Forward line model: start from detector element centers.

Back projection model: start from image pixel centers and interpolate detector element values.

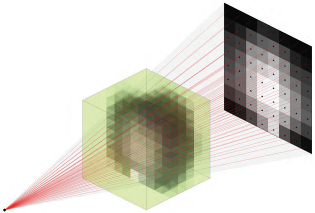
Projectors and Matrices

Multiplication with A $\leftrightsquigarrow$ action of forward projector $\mathcal{R}$.

Multiplication with B $\leftrightsquigarrow$ action of back projector $\mathcal{B}$ = adjoint($\mathcal{R}$).

When we can store A (it is *sparse*), then we can use $B = A^T$, and solve the normal equations $A^T A x = A^T b$ associated with the least squares problem, with x = vec(image) and b = vec(sinogram).

But storage can be problematic. 3D example: 1000 projection angles, 1000×1000 detector elements, $1000 \times 1000 \times 1000$ voxels $\rightarrow$ number of non-zeros in A is of the order 10^{12} $\sim$ several Terabytes of memory.



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

Ray and pixel driven models $\rightarrow$ $B \neq A^T$ $\rightarrow$ unmatched projector pair.

Solve the Unmatched Normal Equations

Classical iterative methods (e.g., Cimmino, SIRT, CGLS) require $B = A^T$. Alternatively, we can solve the **unmatched normal equations**

UNE: $\boxed{B\,A\,x = B\,b}$ or $\boxed{A\,B\,y = b\,, \quad x = B\,y}$

We will use **GMRES** (Saad, Schultz, 1986), a very efficient iterative method for solving systems

$\boxed{M\,x = d}$ with a square and nonsymmetric matrix M.

We skip the implementation details here, and just remind that in the kth step, the iterate x^k of GMRES solves the problem

$$\min_x \|M\,x - d\|_2 \qquad \text{subject to} \qquad x \in \mathcal{K}_k(M, d)\ ,$$

with the *Krylov subspace*

$$\mathcal{K}_k(M, d) = \text{span}\{d,\ Md,\ M^2 d,\ \ldots,\ M^{k-1} d\}\ .$$

AB–GMRES and BA–GMRES

We can formulate *specialized versions* of GMRES for the UNEs:

BA–GMRES solves $B A x = B b$.

AB-GMRES solves $A B y = b, \; x = B y$.

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

Advantages:

- both methods always converge,
- no need for relaxation parameter,
- fairly simple to implement $\rightarrow$ next page.

▷ K. Hayami, J.-F. Yin, T. Ito, *GMRES methods for least squares problems*, SIAM J. Matrix Anal. Appl., 31 (2010), 2400–2430.

▷ H, K. Hayami, K. Morikuni, *GMRES methods for tomographic reconstruction with an unmatched back projector*, J. Comp. Appl. Math., 413 (2022), 114352.

The ABBA Algorithms

Algorithm AB-GMRES

Choose initial x_0
$r_0 = b - A\,x_0$
$w_1 = r_0/\|r_0\|_2$
for $k = 1, 2, \ldots$
$\quad q_k = AB\,w_k$
$\quad$ for $i = 1, 2, \ldots, k$
$\quad\quad h_{i,k} = q_k^T w_i$
$\quad\quad q_k = q_k - h_{i,k}\,w_i$
$\quad$ endfor
$\quad h_{k+1,k} = \|q_k\|_2$
$\quad w_{k+1} = q_k/h_{k+1,k}$
$\quad y_k = \arg\min_y \|\,\|r_0\|_2\,e_1 - H_k\,y\,\|_2$
$\quad x_k = x_0 + B\,[w_1, w_2, \ldots, w_k]\,y_k$
$\quad r_k = b - A\,x_k$
$\quad$ stopping rule goes here
endfor

Algorithm BA-GMRES

Choose initial x_0
$r_0 = B\,b - B\,A\,x_0$
$w_1 = r_0/\|r_0\|_2$
for $k = 1, 2, \ldots$
$\quad q_k = B\,A\,w_k$
$\quad$ for $i = 1, 2, \ldots, k$
$\quad\quad h_{i,k} = q_k^T w_i$
$\quad\quad q_k = q_k - h_{i,k}\,w_i$
$\quad$ endfor
$\quad h_{k+1,k} = \|q_k\|_2$
$\quad w_{k+1} = q_k/h_{k+1,k}$
$\quad y_k = \arg\min_y \|\,\|r_0\|_2\,e_1 - H_k\,y\,\|_2$
$\quad x_k = x_0 + [w_1, w_2, \ldots, w_k]\,y_k$
$\quad r_k = b - A\,x_k$
$\quad$ stopping rule goes here
endfor

MATLAB and Python software available from PCH at
https://people.compute.dtu.dk/pcha/ABBA
and in TIGRE: Tomographic Iterative GPU-based Reconstruction Toolbox
https://github.com/CERN/TIGRE

Obligatory Slide with Many Equations

Hayami, Yin, Ito (2010), H, Hayami, Morikuni (2022)

<u>AB–GMRES</u> solves $\min_y \|A\,B\,y - b\|_2$, $x = B\,y$

- ▷ $\min_x \|A\,x - b\|_2 = \min_y \|A\,B\,y - b\|_2$ holds for all b if an only if $\mathrm{range}(A\,B) = \mathrm{range}(A)$, e.g., if $\mathrm{range}(B) = \mathrm{range}(A^T)$.
- ▷ Monotonic decay of $\|A\,x^k - b\|_2$.
- ▷ Equivalent to LSQR when $B = A^T$.

<u>BA–GMRES</u> solves $\min_x \|B\,A\,x - B\,b\|_2$

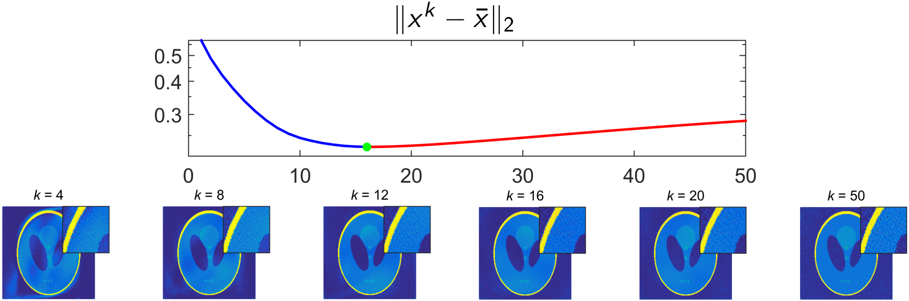
- ▷ the problems $\min_x \|A\,x - b\|_2$ and $\min_x \|B\,A\,x - B\,b\|_2$ are equivalent for all b if and only if $\mathrm{range}(B^T B\,A) = \mathrm{range}(A)$, e.g., if $\mathrm{range}(B^T) = \mathrm{range}(A)$.
- ▷ Monotonic decay of $\|B\,A\,x^k - B\,b\|_2$.
- ▷ Equivalent to LSMR when $B = A^T$.

Conditions are difficult/impossible to check in a given CT problem.

Iterative Methods: Noisy Data Gives Semi-Convergence

The right-hand side b (the data) is a sum of noise-free data $\bar{b} = A\,\bar{x}$ from the ground-truth image $\bar{x}$ plus a noise component e:

$$b = A\,\bar{x} + e, \qquad \bar{x} = \text{ground truth}, \qquad e = \text{noise}.$$

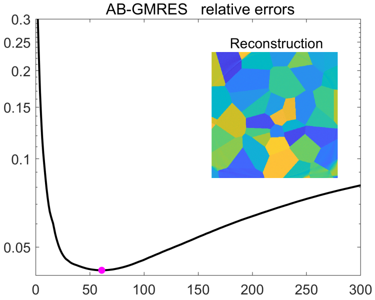


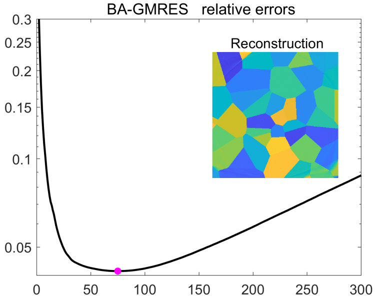
- In the initial iterations x^k approaches the unknown ground truth $\bar{x}$.
- During later iterations x^k converges to the undesired $x^{\text{naïve}} = A^{-1} b$.
- Stop the iterations when the convergence behavior changes.

ABBA Reconstruction Errors $\|x^k - \bar{x}\|_2 / \|\bar{x}\|_2$

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

A and B generated with GPU-ASTRA software; A is $252\,000 \times 176\,400$.



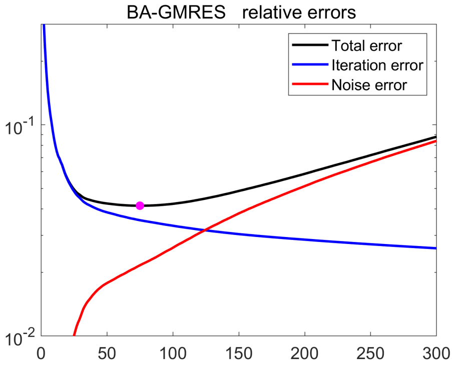


- Semi-convergence is evident for both methods.
- Same minimum reconstruction error $\|x^k - \bar{x}\|_2 / \|\bar{x}\|_2 \approx 0.042$ for both.
- Slightly fewer iterations for AB–GMRES in this example.
- Storage for Krylov bases – AB–GMRES: $m \times k$ – BA–GMRES: $n \times k$.

Error Propagation in BA-GMRES

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

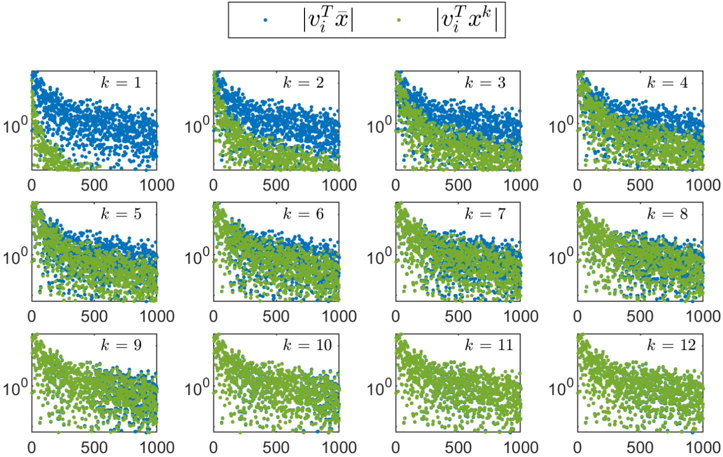
$$\underbrace{x^k - \bar{x}}_{\text{total error}} = \underbrace{x^k - \bar{x}^k}_{\text{noise error}} + \underbrace{\bar{x}^k - \bar{x}}_{\text{iteration error}}$$



Both errors are monotonic in this example – but no guarantee for this.

Semi-Convergence of BA–GMRES ★ SVD Insight

Recall: $b = A\,\bar{x} + e$, $\bar{x}$ = ground truth, $\|e\|_2/\|\bar{b}\|_2 = 0.001$ Gaussian.



- As k increases we capture more and more SVD components in x^k.
- At $k = 11$ we already capture the first 1000 SVD components.

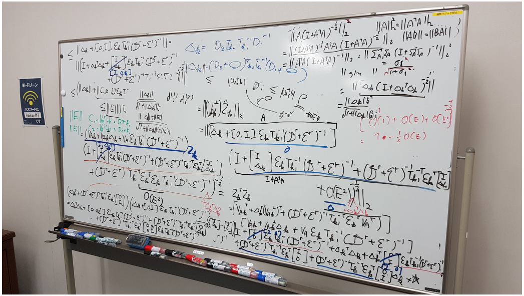
Semi-Convergence of BA–GMRES ★ Subspaces

In our numerical example, $\|B - A^T\|_F / \|B\|_F \approx 0.15$.

So how come we can still compute good reconstructions?

- Compare the Krylov subspace with the SVD subspace.

We are working on it . . .



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:

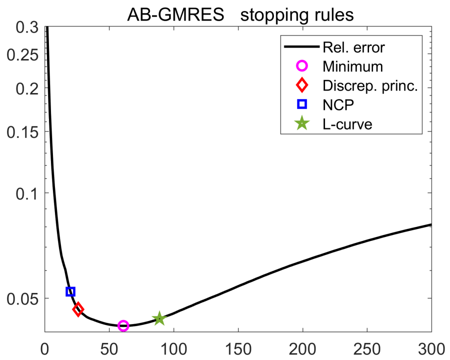
  $$k_{\text{DP}} = \text{the smallest } k \text{ for which } \|b - A\,x^k\|_2 \leq \tau\,\|e\|_2$$

  where $\tau \geq 1$ = 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 $b - A\,x^k$ and identifies when the residual is close to being white noise – which indicates that all available information has been extracted from the noisy data.

- **L-curve criterion:** locates the "corner" of the L-shaped point set $\big(\log\|b - A\,x^k\|_2\,,\ \log\|x^k\|_2\,\big)$.

Stopping Rules in Action



Both the discrepancy principle and the NCP criterion stop too early.

The L-curve criterion stops too late.

A topic for further research, related to all iterative regularization methods.

7th International Conference on Image Formation in X-Ray Computed Tomography, June 12–16, 2022, Baltimore, USA

Computational experiments with real data by:

Emil Y. Sidky, Department of Radiology, University of Chicago.

- Cone-beam CT data from an Epica Pegaso veterinary CT scanner.
- 180 projections taken uniformly over one circular rotation.
- Physical "quality assurance" (QA) phantom $\longrightarrow$
- Detector: 1088×896 pixels of size $(0.278\text{mm})^2$.
- 3D reconstruction: $1024 \times 1024 \times 300$ voxel grid.

Ray-driven projector A. Two choices of B:

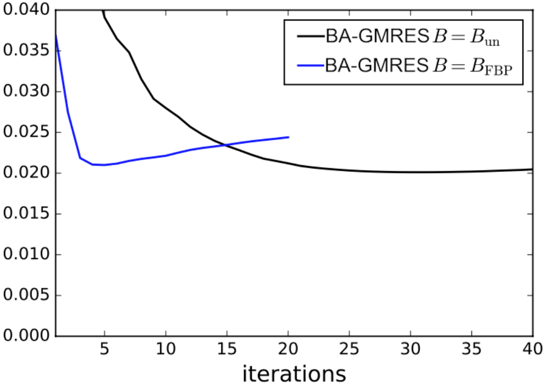
- B_{un} = voxel-driven back projection, linear interpolation on detector.
- $B_{\text{FBP}} = B_{\text{un}} F$ = filtered back-projection, where F = ramp filter.

"Reconstruction Error"

Real data from a physical phantom $\Rightarrow$ no ground truth $\bar{x}$.

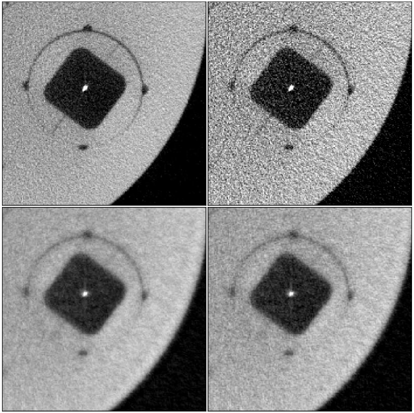
Instead we use a high-quality FBP reconstruction x_{FBP}.

$$\|x^k - x_{\mathrm{FBP}}\|_2$$



With both B-matrices we observe semi-convergence.

Reconstruction, Mid-Slice Region of Interest

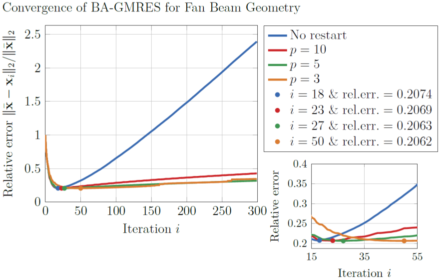


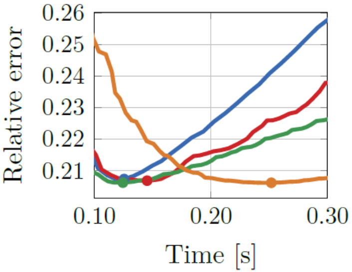
Top left: reference x_{FBP} = FBP reconstructed image from 720 views.
Top right: FBP reconstructed images from 180 views.
Bottom left: BA–GMRES image, $B = B_{\text{un}}$, $k = 29$ iterations, 180 views.
Bottom right: BA–GMRES image, $B = B_{\text{FBP}}$, $k = 4$ iterations, 180 views.

Epilogue: Restart of the ABBA Methods

Must compute and store the orthonormal basis for the Krylov subspace. But orthonormalization is time consuming, and storage may be prohibitive.

Restart solves these problems; more iterations are necessary, but the computing time does not deteriorate.





M. Knudsen, *ABBA Iterative Methods for X-Ray Computed Tomography*, MSc Thesis, DTU, 2023 link

Conclusion

Unmatched projector pairs*

- Need efficient iterative reconstruction methods for unmatched pairs.
- Modify a classical method, e.g., as in the Shifted BA Iteration.
- Use a method that solves the unmatched normal equations $\rightarrow$ ABBA.

*New matched pair: K. Bredies & R. Huber, *Convergence analysis of pixel-driven Radon and fanbeam transforms*, SIAM J. Numer. Anal., 59 (2021), 1399–1432.

Convergence

- Good understanding of convergence for noise-free data.
- Emerging: understanding of semi-convergence for noisy data.

Future

- More theory about semi-convergence for GMRES.

Appendix: Semi-Convergence ★ Technical Insight

Semi-convergence of CGLS is well understood; but only few results have been obtained for GMRES.

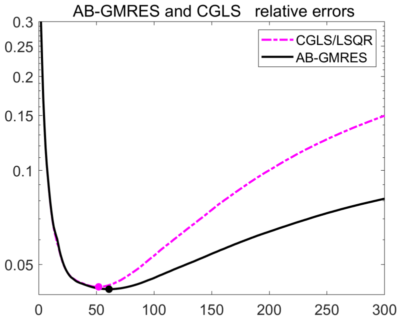
- **Calvetti, Lewis, Reichel (2002):** if the noise-free data lies in a finite-dimensional Krylov subspace, and if GMRES is equipped with a suitable stopping rule, then the GMRES-solution tends towards the exact solution $\bar{x}$ as the noise goes to zero.
- **Gazzola, Novati (2016):** if the discrete Picard condition (DPC) is satisfied 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.

The difficulty is that we cannot analyze GMRES by means of the SVD of A.

A complete understanding has not emerged yet. Here we rely on some preliminary analysis and insight from numerical experiments.

Appendix: Comparison with CGLS/LSQR and LSMR

If $B = A^T$ then AB–GMRES = CGLS/LSQR and BA–GMRES = LSMR.



Recall: for large-scale problems we do not have a choice; we must use B.

The good news is that the reconstruction error does not deteriorate, compared with using A^T (in this example, the error is slightly smaller).