

Regularization of large discrete inverse problems by iterative projection methods

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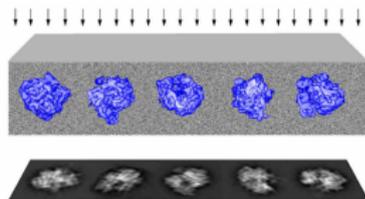
SNA 21 - January 2021

Outline

1. Inverse problems
2. Regularization by projection
3. Propagation of noise
4. Analysis of residuals
5. Hybrid methods
6. Conclusion

3D Example: Electron microscopy

$$PSF_{\omega} * (P_{\omega}f + e_{\omega}^s) + e_{\omega}^b = g_{\omega}$$



- f : Unknown function representing the particle
- ω : Projection angle.
- PSF_{ω} : Point Spread Function.
- P_{ω} : X-Ray transform: $P_{\omega}f(s) := \int_{-\infty}^{\infty} f(t \cdot \omega + s)dt$, $s \in \omega^{\perp}$.
- $e_{\omega}^s, e_{\omega}^b$: Structure and background noise functions.
- g_{ω} : Measured data.
- $*$: Convolution operator.

Discrete model (one projection)

$$PSF_{\omega} * (P_{\omega} f + e_{\omega}^s) + e_{\omega}^b = g_{\omega} \quad \text{Continuous model}$$

$$C_{\omega} (\bar{P}_{\omega} \bar{f} + \bar{e}_{\omega}^s) + \bar{e}_{\omega}^b = \bar{g}_{\omega} \quad \text{Discrete model}$$

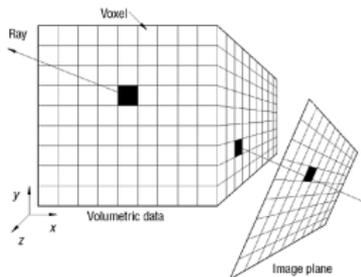


Figure: 3D grid discretization with unknown voxel values.

Linear model

Consider a linear **ill-posed** problem

$$b = Ax + e,$$

where the **noise vector** e

- is an **unknown perturbation** (rounding errors, errors of measurement, noise with physical sources, etc.),
- with the unknown noise level

$$\delta^{\text{noise}} \equiv \|e\|/\|b\| \ll 1$$

Properties of the problem:

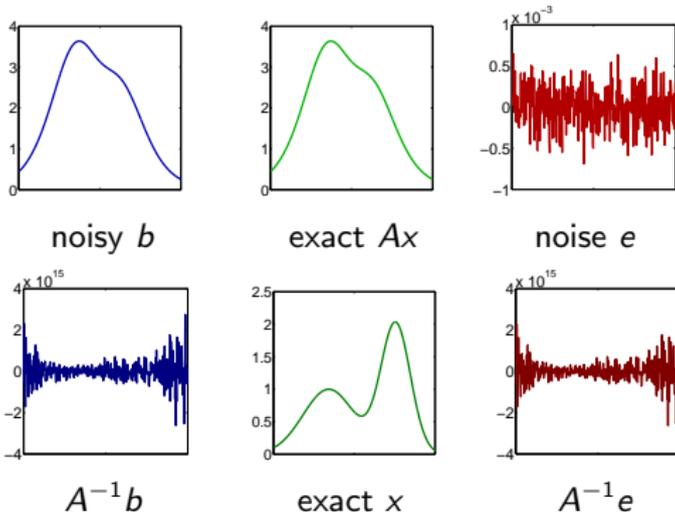
- A dampens high frequencies (smoothing property),
- exact right-hand side is smooth, but noise is not,
- small changes in b cause **large changes in the solution**.

Naive solution - noise amplification

$$b = Ax + e, \quad \text{where } \|Ax\| \gg \|e\| \quad \text{BUT}$$

$$A^{-1}b = x + A^{-1}e, \quad \text{where } \|x\| \ll \|A^{-1}e\|$$

1D Example: shaw(400), $\delta^{\text{noise}} \approx 1e-4$, white noise



Naive solution - noise amplification

Singular value decomposition (SVD): $R = \text{rank}(A)$

$$A = U\Sigma V^T = \sum_{j=1}^R u_j^T \sigma_j v_j,$$

$$\Sigma = \text{diag}\{\sigma_1, \dots, \sigma_R, 0, \dots, 0\},$$

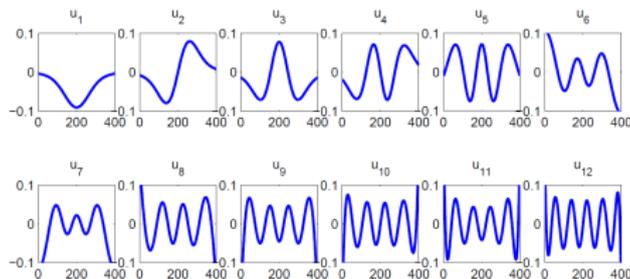
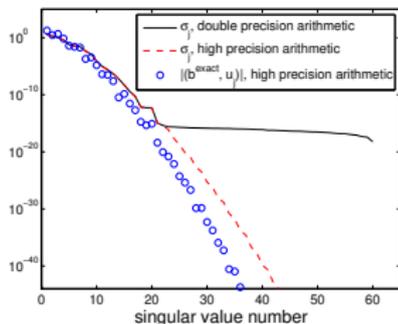
where $U = [u_1, \dots, u_N]$ and $V = [v_1, \dots, v_M]$ are unitary matrices.

Then

$$x^{\text{naive}} \equiv A^\dagger b = \underbrace{\sum_{j=1}^R \frac{u_j^T b^{\text{exact}}}{\sigma_j} v_j}_{x^{\text{exact}}} + \underbrace{\sum_{j=1}^R \frac{u_j^T e}{\sigma_j} v_j}_{\text{noise component}}.$$

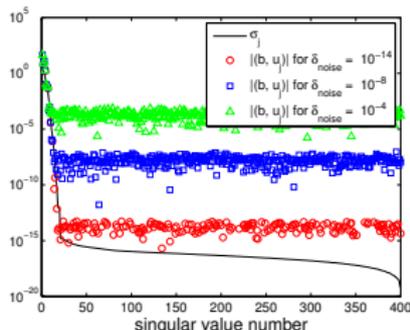
Discrete Picard condition (DPC)

- singular values of A **decay quickly** without a noticeable gap;
- singular vectors u_i, v_j of A represent increasing frequencies;
- for the exact right-hand side, $|(b^{\text{exact}}, u_j)|$ **decay faster** than the singular values σ_j of A (**DPC**)



Noise amplification

White noise: $|(e, u_j)|$, $j = 1, \dots, N$ do not exhibit any trend



$$x^{\text{naive}} \equiv A^\dagger b = \underbrace{\sum_{j=1}^R \frac{u_j^T b^{\text{exact}}}{\sigma_j} v_j}_{x^{\text{exact}}} + \underbrace{\sum_{j=1}^R \frac{u_j^T e}{\sigma_j} v_j}_{\text{amplified noise}}$$

Components corresponding to small σ_j 's are dominated by e^{HF} .

2D imaging problem

For a blurred image B

$$x^{\text{naive}} = \sum_{j=1}^R \underbrace{\frac{u_j^T \text{vec}(B)}{\sigma_j}}_{\text{scalar}} v_j, \quad X = \text{mtx}(x),$$

is a linear combination of right singular vectors v_j .

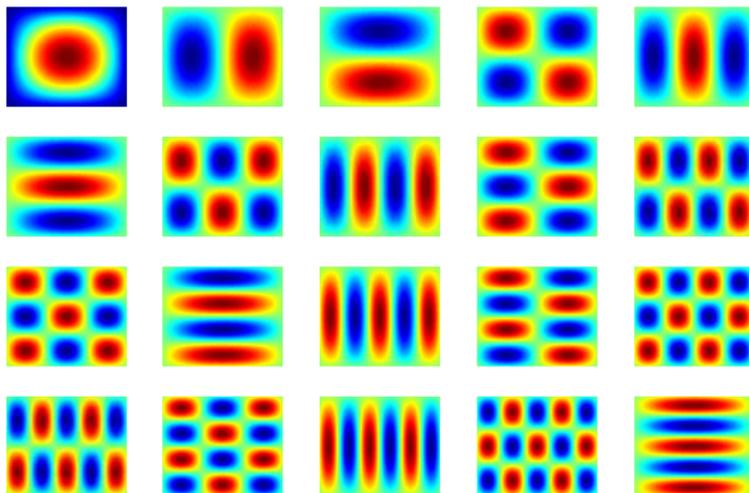
It can be further rewritten as

$$X^{\text{naive}} = \sum_{j=1}^R \frac{u_j^T \text{vec}(B)}{\sigma_j} V_j, \quad V_j = \text{mtx}(v_j) \in \mathbb{R}^{m \times n}$$

using **singular images** V_j (the reshaped right singular vectors).

2D imaging problem: Singular images

Singular images $V_j \in \mathbb{R}^{m \times n}$ for 2D image deblurring model
(Gaussian blur, zero BC, artificial colors).



Filtered solution

Unwanted components can be suppressed by

$$x^{\text{filtered}} = \sum_{j=1}^R \phi_j \frac{u_j^T b}{\sigma_j} v_j, \quad x^{\text{filtered}} = V \Phi \Sigma^{-1} U^T b,$$

where $\Phi = \text{diag}(\phi_1, \dots, \phi_N)$. In image deblurring problem

$$X^{\text{filtered}} = \sum_{j=1}^R \phi_j \frac{u_j^T \text{vec}(B)}{\sigma_j} V_j.$$

The filter factors are given by some filter function

$$\phi_j = \phi(j, A, b, \dots).$$

Classical regularization approaches

Spectral filtering (e.g., truncated SVD, Tikhonov): suitable for solving small ill-posed problems.

Projection on smooth subspaces: suitable for solving large ill-posed problems. The dimension of projection space represents a regularization parameter.

Hybrid techniques: combination of outer iterative regularization with a spectral filtering of the projected small problem.

... etc.

Large scale problems

- Direct filtering of SVD is too costly.
- The method should avoid work with full A .
- The method should take advantage of data properties (sparsity, structure, ...).
- The approximation must be dominated by low frequencies, high frequencies must be dumped.

We try to look for an approximation in some low dimensional subspace \mathcal{W}_k dominated by low frequencies.

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Projection methods

Consider a subspace

$$\mathcal{W}_k = \text{span}(w_1, \dots, w_k) \subset \mathbb{R}^N, \quad W_k = [w_1, \dots, w_k] \in \mathbb{R}^{N \times k},$$

such that $W_k^T W_k = I_k$ and w_j are dominated by low frequencies.

Then we solve the **projected problem**

$$\begin{aligned} \min_{x \in \mathcal{W}_k} \|b - Ax\| &\Leftrightarrow \min_{y \in \mathbb{R}^k} \|b - (AW_k)y\| \\ &\Leftrightarrow W_k^T (A^T A) W_k y = W_k^T A^T b. \end{aligned}$$

The question is, **how to choose the basis** w_j ?

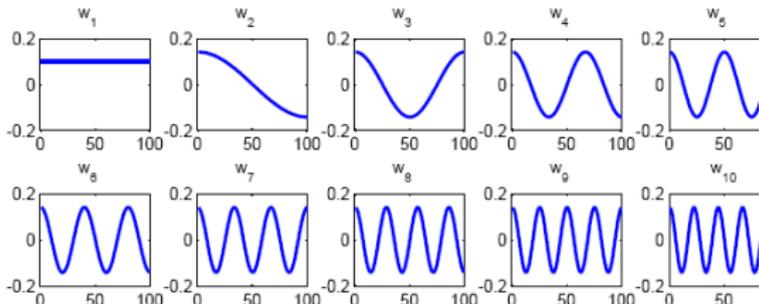
Projection using DCT basis

An example of a suitable basis is the DCT basis

$$w_1 = \sqrt{\frac{1}{N}} (1, 1, \dots, 1)^T,$$

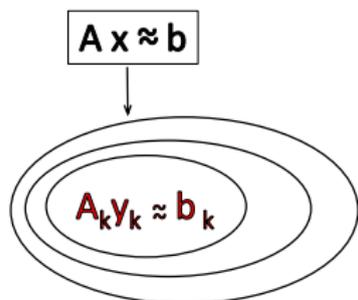
$$w_j = \sqrt{\frac{2}{N}} \left(\cos\left(\frac{(j-1)\pi}{2N}\right), \cos\left(\frac{3(j-1)\pi}{2N}\right), \dots, \cos\left(\frac{(2N-1)(j-1)\pi}{2N}\right) \right)^T,$$

for $j > 1$.



Krylov subspace methods

When A is large/sparse/not given explicitly, approximation by projection onto a **low dimensional Krylov subspace** is advantageous.



$$\mathcal{K}_k(C, d) \equiv \text{Span}\{d, Cd, \dots, C^{k-1}d\}$$

$$\mathcal{K}_1(C, d) \subseteq \mathcal{K}_2(C, d) \subseteq \dots$$

For A square: $\mathcal{K}_k(A, b) \dots$ GMRES, CG, MINRES

$\vec{\mathcal{K}}_k(A, b) \dots$ RRGMRES, MINRES-II

For A general: $\mathcal{K}_k(A^T A, A^T b) \dots$ LSQR, LSMR, CGLS

$$x_k \longrightarrow x^{\text{naive}}$$

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Regularization based on GK

$x_k = W_k y_k$, where the columns of W_k span $\mathcal{K}_k(A^T A, A^T b)$

LSQR method: minimize the residual

$$\min_{x \in \mathcal{K}_k(A^T A, A^T b)} \|Ax - b\| = \min_{y \in \mathbb{R}^k} \|L_{k+} y - \beta_1 e_1\|$$

CRAIG method: minimize the error

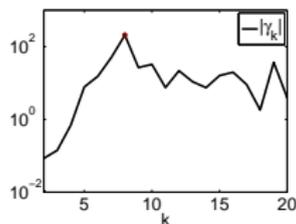
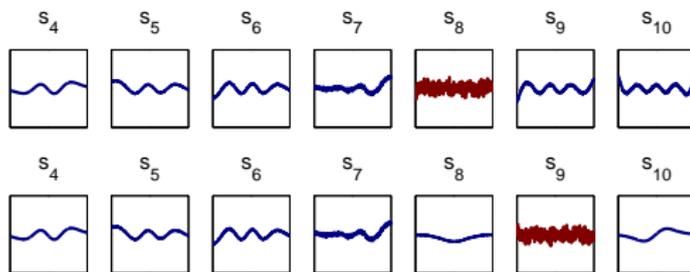
$$\min_{x \in \mathcal{K}_k(A^T A, A^T b)} \|x^* - x\| = \min_{y \in \mathbb{R}^k} \|L_k y - \beta_1 e_1\|$$

LSMR method: minimize $A^T r_k$

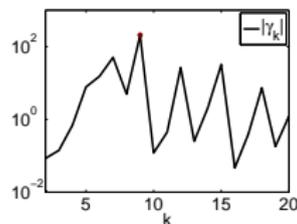
$$\min_{x \in \mathcal{K}_k(A^T A, A^T b)} \|A^T (Ax - b)\| = \min_{y \in \mathbb{R}^k} \|L_{k+1}^T L_{k+} y - \beta_1 \alpha_1 e_1\|$$

Influence of the loss of orthogonality

Comparison GK with and without reorthogonalization:



with ReOG

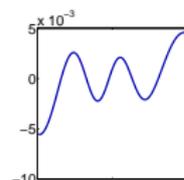
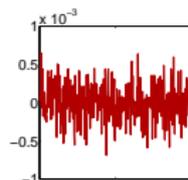
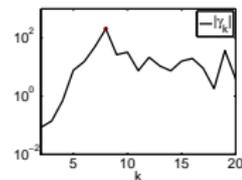


without ReOG

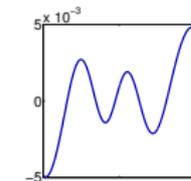
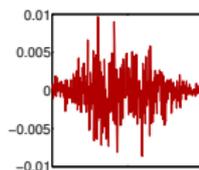
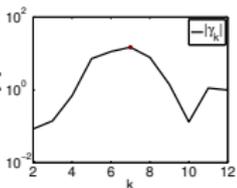
Aggregation may be necessary [Gergelits, H., Kubínová - 18].

Noise estimate for shaw(400)

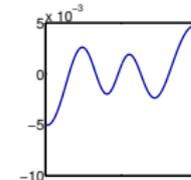
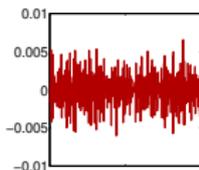
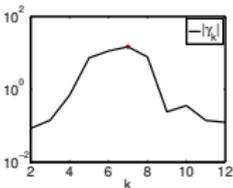
White:



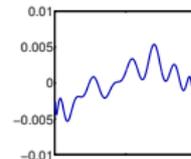
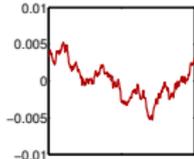
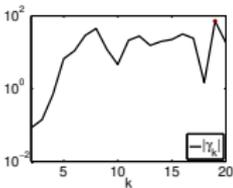
Data correlated:



High-frequency:



Low-frequency:

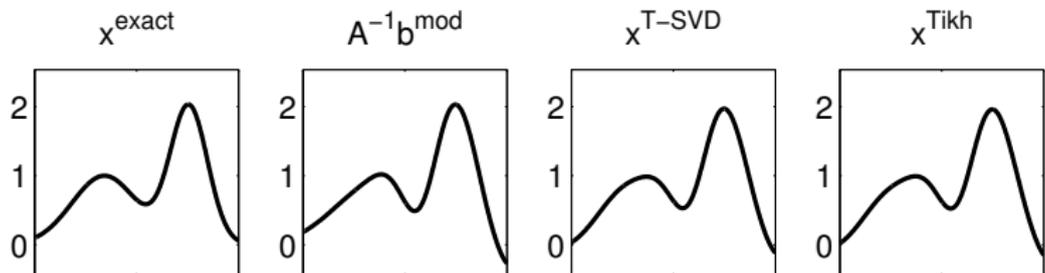


e

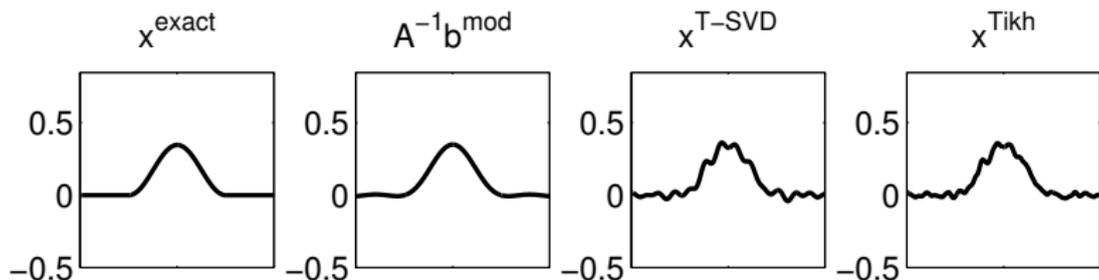
$e - \tilde{e}$

Comparison of noise reduction to spectral filtering

shaw(400), white noise



phillips(400), white noise



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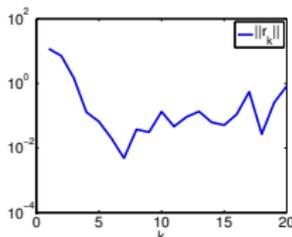
Residual of CRAIG method

$$\min_{x \in \mathcal{K}_k(A^T A, A^T b)} \|x^* - x\| = \min_{y \in \mathbb{R}^k} \|L_k y - \beta_1 e_1\|, \quad x_k = W_k y_k$$

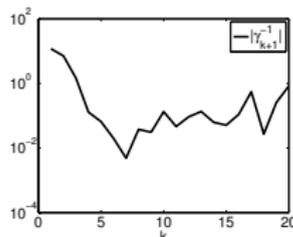
Theorem: x_k^{CRAIG} is the exact solution to the consistent system

$$A x_k^{\text{CRAIG}} = b - \varphi_k(0)^{-1} s_{k+1}.$$

Consequently, $\|r_k^{\text{CRAIG}}\| = |\varphi_k(0)^{-1}| \equiv |\gamma_{k+1}|^{-1}$ reaches its minimum in the noise revealing iteration.



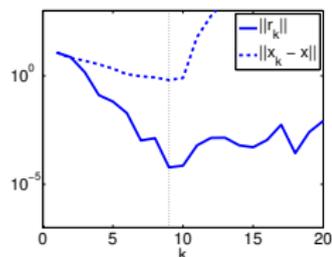
CRAIG residual



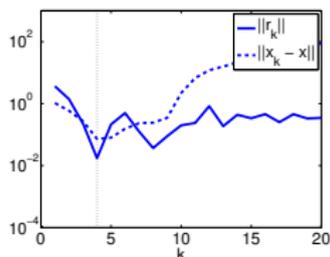
inverted ampl. factor

Comparison of the error and the residual

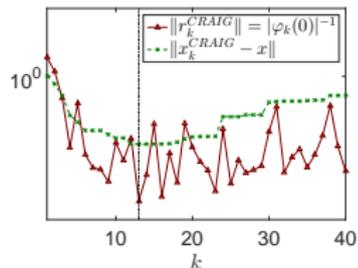
Measuring the **size of the residual** seems to be a **valid stopping criterion** for CRAIG. The **minimal error** is reached approximately at the **iteration with the minimal residual**.



shaw(400)



phillips(1000)



phillips, no ReOG

Residual of LSQR method

$$\min_{x \in \mathcal{K}_k(A^T A, A^T b)} \|Ax - b\| = \min_{y \in \mathbb{R}^k} \|L_{k+} y - \beta_1 e_1\|, \quad x_k = W_k y_k$$

Theorem: The residual corresponding to x_k^{LSQR} satisfies

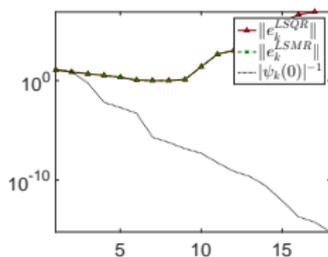
$$r_k^{\text{LSQR}} = \frac{1}{\sum_{l=0}^k \varphi_l(0)^2} \sum_{l=0}^k \varphi_l(0) s_{l+1}.$$

Consequently, the **size of the component** of r_k in the direction of s_j is **proportional to the amount of propagated noise e^{HF} in s_j .**

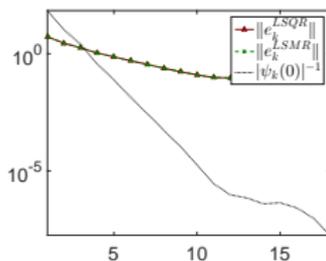
Residual of LSMR method

$$\min_{x \in \mathcal{K}_k(A^T A, A^T b)} \|A^T(Ax - b)\| = \min_{y \in \mathbb{R}^k} \|L_{k+1}^T L_k y - \beta_1 \alpha_1 e_1\|$$

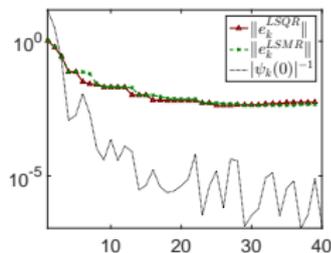
Components of r_k in LSMR behave similarly as in LSQR. The errors resemble as long as $|\psi_k(0)|$ (the absolute term of the Lanczos polynomial for GK vectors w_k) grows rapidly.



shaw(400), white

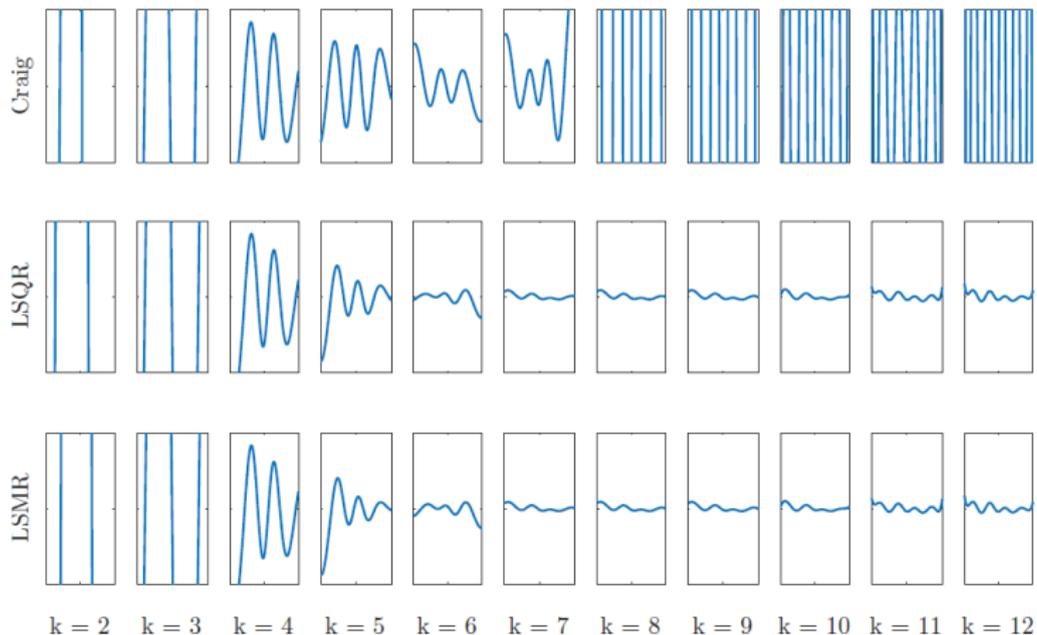


gravity(400), Poisson

phillips(400),
white, no ReOG

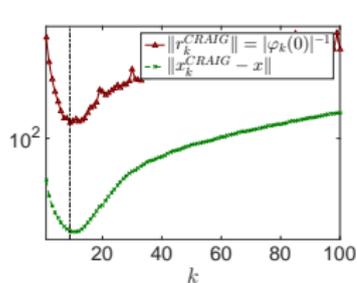
Comparison of noise and residuals

$$e - r_k, \text{ shaw, } \delta_{\text{noise}} = 0.001$$

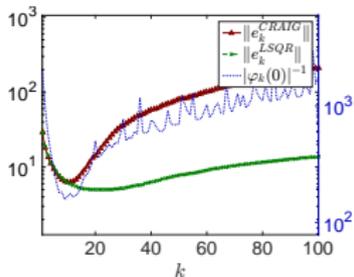


Comparison of the methods - large 2D problems

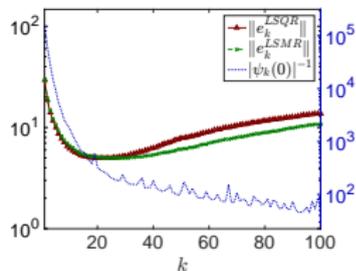
Example: seismictomo(100,100,200), white noise,
 $\delta_{\text{noise}} = 0.01$, $A \in \mathbb{R}^{20000 \times 10000}$, no ReOG



CRAIG error and residual



CRAIG vs LSQR

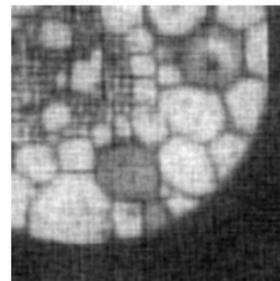
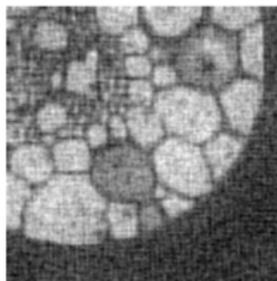
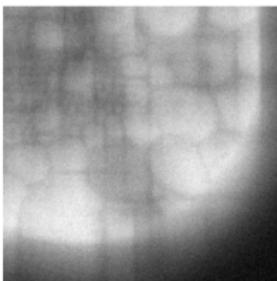
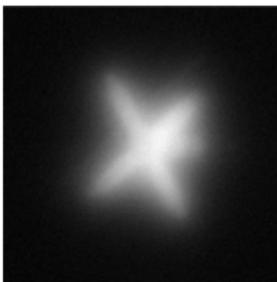


LSQR vs LSMR

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2D image deblurring - reconstructions



Blurred & 5% noise

LSMR

hybrid LSMR

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Selected references

Software:

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- P. C. Hansen, and J. S. Jrgensen: AIR Tools II Version 1.0, 2018.
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- M. Hanke: A Taste of Inverse Problems: Basic Theory and Examples, SIAM, 2017.
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- P. C. Hansen, J. G. Nagy, and D. P. O'Leary: Deblurring Images: Matrices, Spectra, and Filtering, SIAM, 2006.

**Thank you for your
attention!**