Flexible Krylov Methods for ℓ_p Regularization

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Joint work with **Julianne Chung** and **Malena Sabaté Landman**

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UNIVERSITY OF BATH

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What is this talk about?

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Regularization of linear inverse problems

$$\mathbf{A}\mathbf{x}_{\mathrm{true}} + \boldsymbol{\epsilon} = \mathbf{b}\,,$$

where

$\mathbf{b} \in \mathbb{R}^M$	observations or measurements
$\mathbf{x}_{\mathrm{true}} \in \mathbb{R}^N$	desired parameters
$\mathbf{A} \in \mathbb{R}^{M\times N}$	ill-conditioned matrix models forward process
$\boldsymbol{\epsilon} \in \mathbb{R}^M$	additive Gaussian noise

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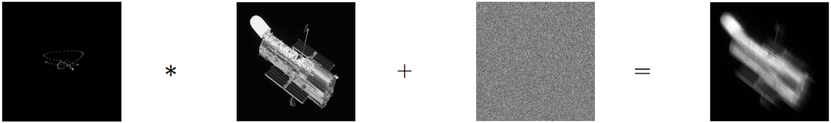
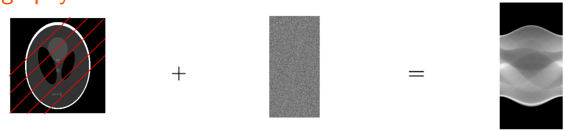
image deblurring and denoising



computed tomography



Outline

Applying variational regularization...

$$\mathbf{x}^{\mathrm{reg}} = \arg\min_{\mathbf{x}\in\mathbb{R}^N} \|\mathbf{A}\mathbf{x}-\mathbf{b}\|_2^2 + \lambda\mathcal{R}(\mathbf{x}), \quad \lambda > 0$$

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$$\mathbf{A}\mathbf{Z}_k = \mathbf{W}_{k+1}\mathbf{G}_k$$

$$\mathbf{x}_k = \mathbf{Z}_k\mathbf{y}_k, \quad \mathbf{y}_k = \arg\min_{\mathbf{y}\in\mathbb{R}^k} \|\mathbf{g}_k - \mathbf{G}_k\mathbf{y}\|_2^2$$

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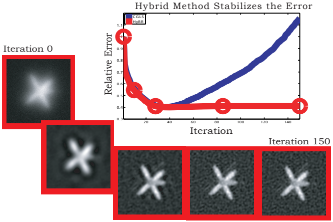
Fast semi-convergence



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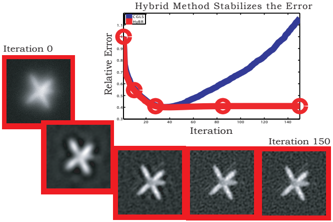

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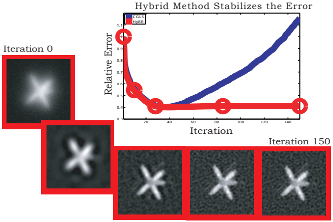

Fast semi-convergence

Hanke (1995); Frommer and Maas (1999);
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Kilmer, Hansen, Espanol (2007); Chung and Palmer (2015); G., Novati, Russo (2015)
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- ℓ^p regularization
  (we will consider $\mathcal{R}(\mathbf{x}) = \|\mathbf{x}\|_p^p$, $\mathcal{R}(\mathbf{x}) = \|\mathbf{\Psi}\mathbf{x}\|_p^p$, $\mathcal{R}(\mathbf{x}) = \mathrm{TV}_p(\mathbf{x})$; $p \geq 1$, $p > 0$)

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  - Constrained optimization
    Chen et al (1999), Bertsekas (2004), Gafni and Bertsekas (1984), ...
  - Iterative shinkage-thresholding algorithms (ISTA)
    Bioucas-Dias and Figueiredo(2007), Giryes, Elad and Eldar (2011), Beck and Teboulle (2009), Goldstein and Osher (2009), Osher et al (2005) ....
  - Iteratively re-weighted norm
    Rodriguez and Wohlberg (2008), Renaut et al (2017), ...
  - Generalized Krylov methods for $\ell_p - \ell_q$
    Lanza et al (2015), Huang, Lanza, Morigi, Reichel, Sgallari (2017), Buccini and Reichel (2019),...
  - Flexible Arnoldi methods (for square problems)
    Gazzola and Nagy (2014)
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IRN algorithm

Input: $\mathbf{A}$, $\mathbf{b}$, $\mathbf{x}_0 (= 0)$, $\mathbf{L}_0 = \mathbf{L}(\mathbf{x}_0) (= \mathbf{I})$

- For $k = 1, \dots,$ till a stopping criterion is satisfied

$$\mathbf{x}_k = \arg\min_{\mathbf{x} \in \mathbb{R}^N} \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_2^2 + \lambda \|\mathbf{L}_{k-1}\mathbf{x}\|_2^2$$

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... revisited within Flexible Krylov methods ...

[G. and Nagy (2014)]

1. For $\mathbf{A} \in \mathbb{R}^{N \times N}$, use *flexible* Arnoldi to generate basis vectors: [Saad (1993, 2003)]

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Flexible Golub-Kahan (FGK) Process

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A new flexible factorization

Flexible Golub-Kahan (FGK) Process

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Given $\mathbf{A} \in \mathbb{R}^{M\times N}, \mathbf{b} \in \mathbb{R}^{M}$, initialize $\mathbf{u}_1 = \mathbf{b}/\beta_1$ where $\beta_1 = \|\mathbf{b}\|$.

After k iterations with changing preconditioners $\mathbf{L}_k$, we have

Related to inexact Krylov methods [Simoncini and Szyld (2007)]

- $\mathbf{Z}_k = \begin{bmatrix} \mathbf{L}_1^{-1}\mathbf{v}_1 & \cdots & \mathbf{L}_k^{-1}\mathbf{v}_k \end{bmatrix} \in \mathbb{R}^{N\times k}$
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such that

$$\mathbf{A}\mathbf{Z}_k = \mathbf{U}_{k+1}\mathbf{M}_k \quad \text{and} \quad \mathbf{A}^\top\mathbf{U}_{k+1} = \mathbf{V}_{k+1}\mathbf{T}_{k+1}$$

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Remarks:

- If $\mathbf{L}_k = \mathbf{L}$, get right-preconditioned GK bidiagonalization
- Additional orthogonalizations and storage

Flexible LSQR and flexible LSMR

New flexible solvers

Flexible LSQR and flexible LSMR

1. Use *flexible* GK to generate basis vectors:

$$\mathbf{Z}_k = \begin{bmatrix} \mathbf{L}_1^{-1}\mathbf{v}_1 & \cdots & \mathbf{L}_k^{-1}\mathbf{v}_k \end{bmatrix} \in \mathbb{R}^{n\times k}$$

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2. Compute solution $\mathbf{x}_k = \mathbf{Z}_k\mathbf{y}_k$ where
   - Flexible LSQR (FLSQR)

$$\mathbf{y}_k = \arg\min_{\mathbf{y}\in\mathbb{R}^k} \|\mathbf{M}_k\mathbf{y} - \beta_1\mathbf{e}_1\|_2^2$$

   - Flexible LSMR (FLSMR)

$$\mathbf{y}_k = \arg\min_{\mathbf{y}\in\mathbb{R}^k} \|\mathbf{T}_{k+1}\mathbf{M}_k\mathbf{y} - \beta_1 m_{11}\mathbf{e}_1\|_2^2$$

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     Optimality property:

     $\mathbf{x}_k$ minimizes $\|\mathbf{A}\mathbf{x}_k - \mathbf{b}\|_2$ over $\mathbf{x}_0 + \mathrm{span}\{\mathbf{Z}_k\}$.

   - Flexible LSMR (FLSMR)

$$\mathbf{y}_k = \arg\min_{\mathbf{y}\in\mathbb{R}^k} \|\mathbf{T}_{k+1}\mathbf{M}_k\mathbf{y} - \beta_1 m_{11}\mathbf{e}_1\|_2^2$$

Flexible LSQR and flexible LSMR

1. Use *flexible* GK to generate basis vectors:

$$\mathbf{Z}_k = \begin{bmatrix} \mathbf{L}_1^{-1}\mathbf{v}_1 & \cdots & \mathbf{L}_k^{-1}\mathbf{v}_k \end{bmatrix} \in \mathbb{R}^{n\times k}$$

$$\mathbf{A}\mathbf{Z}_k = \mathbf{U}_{k+1}\mathbf{M}_k \quad \text{and} \quad \mathbf{A}^\top \mathbf{U}_{k+1} = \mathbf{V}_{k+1}\mathbf{T}_{k+1}$$

2. Compute solution $\mathbf{x}_k = \mathbf{Z}_k\mathbf{y}_k$ where
   - Flexible LSQR (FLSQR)

$$\mathbf{y}_k = \arg\min_{\mathbf{y}\in\mathbb{R}^k} \|\mathbf{M}_k\mathbf{y} - \beta_1\mathbf{e}_1\|_2^2$$

Optimality property:

$\mathbf{x}_k$ minimizes $\|\mathbf{A}\mathbf{x}_k - \mathbf{b}\|_2$ over $\mathbf{x}_0 + \mathrm{span}\{\mathbf{Z}_k\}$.

   - Flexible LSMR (FLSMR)

$$\mathbf{y}_k = \arg\min_{\mathbf{y}\in\mathbb{R}^k} \|\mathbf{T}_{k+1}\mathbf{M}_k\mathbf{y} - \beta_1 m_{11}\mathbf{e}_1\|_2^2$$

Optimality property:
$\mathbf{x}_k$ minimizes $\left\|\mathbf{A}^\top(\mathbf{A}\mathbf{x}_k - \mathbf{b})\right\|_2$ over $\mathbf{x}_0 + \mathrm{span}\{\mathbf{Z}_k\}$.
Equivalency result:
FLSMR is equivalent to FGMRES applied to the normal equations.

Flexible GK (FGK) *hybrid* methods

New flexible solvers
used in a hybrid framework

Flexible GK (FGK) *hybrid* methods

1. Use *flexible* GK to generate basis vectors:

$$\mathbf{Z}_k = \left[\mathbf{L}_1^{-1}\mathbf{v}_1 \quad \cdots \quad \mathbf{L}_k^{-1}\mathbf{v}_k\right] \in \mathbb{R}^{N\times k}$$

$$\mathbf{A}\mathbf{Z}_k = \mathbf{U}_{k+1}\mathbf{M}_k \quad \text{and} \quad \mathbf{A}^\top\mathbf{U}_{k+1} = \mathbf{V}_{k+1}\mathbf{T}_{k+1}$$

Flexible GK (FGK) *hybrid* methods

1. Use *flexible* GK to generate basis vectors:

$$\mathbf{Z}_k = \begin{bmatrix} \mathbf{L}_1^{-1}\mathbf{v}_1 & \cdots & \mathbf{L}_k^{-1}\mathbf{v}_k \end{bmatrix} \in \mathbb{R}^{N\times k}$$

$$\mathbf{A}\mathbf{Z}_k = \mathbf{U}_{k+1}\mathbf{M}_k \quad \text{and} \quad \mathbf{A}^\top\mathbf{U}_{k+1} = \mathbf{V}_{k+1}\mathbf{T}_{k+1}$$

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2. Compute solution $\mathbf{x}_k = \mathbf{Z}_k\mathbf{y}_k$, where
   - Flexible GK Tikhonov - R (FLSQR-R)

$$\mathbf{y}_k = \arg\min_{\mathbf{y}\in\mathbb{R}^k} \left\|\mathbf{M}_k\mathbf{y} - \beta_1\mathbf{e}_1\right\|_2^2 + \lambda_k \left\|\mathbf{R}_k\mathbf{y}\right\|_2^2 , \quad \mathbf{Z}_k = \mathbf{Q}_k\mathbf{R}_k$$

Flexible GK (FGK) *hybrid* methods

1. Use *flexible* GK to generate basis vectors:

$$\mathbf{Z}_k = \begin{bmatrix} \mathbf{L}_1^{-1}\mathbf{v}_1 & \cdots & \mathbf{L}_k^{-1}\mathbf{v}_k \end{bmatrix} \in \mathbb{R}^{N \times k}$$

$$\mathbf{A}\mathbf{Z}_k = \mathbf{U}_{k+1}\mathbf{M}_k \quad \text{and} \quad \mathbf{A}^\top \mathbf{U}_{k+1} = \mathbf{V}_{k+1}\mathbf{T}_{k+1}$$

2. Compute solution $\mathbf{x}_k = \mathbf{Z}_k\mathbf{y}_k$, where
   - Flexible GK Tikhonov - R (FLSQR-R)

$$\mathbf{y}_k = \arg\min_{\mathbf{y}\in\mathbb{R}^k} \|\mathbf{M}_k\mathbf{y} - \beta_1\mathbf{e}_1\|_2^2 + \lambda_k \|\mathbf{R}_k\mathbf{y}\|_2^2 \,, \quad \mathbf{Z}_k = \mathbf{Q}_k\mathbf{R}_k$$

   - Flexible GK Tikhonov - I (FLSQR-I)

$$\mathbf{y}_k = \arg\min_{\mathbf{y}\in\mathbb{R}^k} \|\mathbf{M}_k\mathbf{y} - \beta_1\mathbf{e}_1\|_2^2 + \lambda_k \|\mathbf{y}\|_2^2$$

FLSQR-R: Approximate singular values of $\mathbf{A}$

$$\mathbf{R}_k^{-\top}\mathbf{M}_k^{\top}\mathbf{M}_k\mathbf{R}_k^{-1} = \mathbf{R}_k^{-\top}\mathbf{M}_k^{\top}\mathbf{U}_{k+1}^{\top}\mathbf{U}_{k+1}\mathbf{M}_k\mathbf{R}_k^{-1} = \mathbf{Q}_k^{\top}\mathbf{A}^{\top}\mathbf{A}\mathbf{Q}_k$$

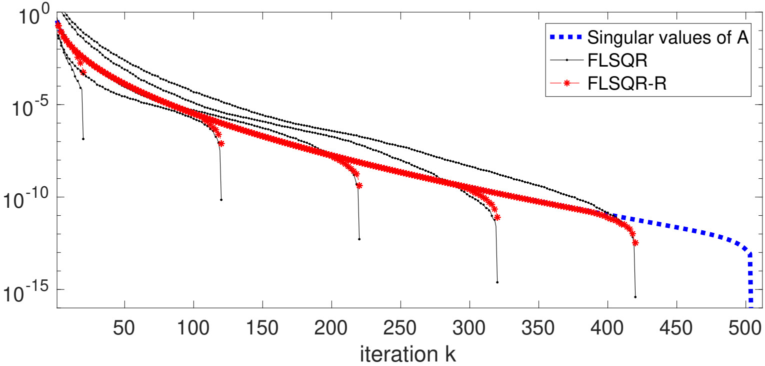

Figure: This plot compares the singular values of $\mathbf{A}$ to the singular values of $\mathbf{M}_k$ from FLSQR and of $\mathbf{M}_k\mathbf{R}_k^{-1}$ from FLSQR-R, for iterations k between 20 and 420 in increments of 100.

Solving the transformed problem

Let $\mathbf{\Psi} \neq \mathbf{I}$ (invertible), $p = 1$ (e.g., $\mathbf{\Psi}$: image domain $\rightarrow$ wavelet domain)

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Equivalent problems (for $\widetilde{\mathbf{\Psi}}$ orthogonal):

[Belge, Kilmer, Miller (2000)]

$$\min_{\mathbf{x}\in\mathbb{R}^N} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2 + \lambda \|\mathbf{\Psi}\mathbf{x}\|_1 \Leftrightarrow \min_{\mathbf{x}\in\mathbb{R}^N} \|\underbrace{\widetilde{\mathbf{\Psi}}\mathbf{A}\mathbf{\Psi}^{-1}}_{\mathbf{H}}\underbrace{\mathbf{\Psi}\mathbf{x}}_{\mathbf{s}} - \underbrace{\widetilde{\mathbf{\Psi}}\mathbf{b}}_{\mathbf{d}}\|_2^2 + \lambda\|\underbrace{\mathbf{\Psi}\mathbf{x}}_{\mathbf{s}}\|_1$$

Solution subspace for flexible Arnoldi:

$$\mathbf{s}_k \in \mathrm{span}\{\mathbf{L}_1^{-1}\widehat{\mathbf{v}}_1, \mathbf{L}_2^{-1}\widehat{\mathbf{v}}_2, \dots, \mathbf{L}_k^{-1}\widehat{\mathbf{v}}_k\}, \quad \text{where} \quad \begin{array}{rcl} \widehat{\mathbf{v}}_1 & = & \mathbf{d}/\|\mathbf{d}\|_2 \\ \widehat{\mathbf{v}}_2 & = & \mathrm{ONC}(\mathbf{H}\mathbf{L}_1^{-1}\widehat{\mathbf{v}}_1) \\ \widehat{\mathbf{v}}_3 & = & \mathrm{ONC}(\mathbf{H}\mathbf{L}_2^{-1}\widehat{\mathbf{v}}_2) \\ \dots & & \end{array}$$

Solving the transformed problem

Let $\boldsymbol{\Psi} \neq \mathbf{I}$ (invertible), $p = 1$ (e.g., $\boldsymbol{\Psi}$: image domain $\rightarrow$ wavelet domain)
Equivalent problems (for $\widetilde{\boldsymbol{\Psi}}$ orthogonal):
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$$\mathbf{x}_k = \boldsymbol{\Psi}^{-1}\mathbf{s}_k$$

Solving the transformed problem

Let $\mathbf{\Psi} \neq \mathbf{I}$ (invertible), $p = 1$ (e.g., $\mathbf{\Psi}$: image domain $\rightarrow$ wavelet domain)
Equivalent problems (for $\widetilde{\mathbf{\Psi}}$ orthogonal):
[Belge, Kilmer, Miller (2000)]

$$\min_{\mathbf{x}\in\mathbb{R}^N} \|\mathbf{Ax} - \mathbf{b}\|_2^2 + \lambda \|\mathbf{\Psi x}\|_1 \Leftrightarrow \min_{\mathbf{x}\in\mathbb{R}^N} \|\underbrace{\widetilde{\mathbf{\Psi}}\mathbf{A}\mathbf{\Psi}^{-1}}_{\mathbf{H}}\underbrace{\mathbf{\Psi x}}_{\mathbf{s}} - \underbrace{\widetilde{\mathbf{\Psi}}\mathbf{b}}_{\mathbf{d}}\|_2^2 + \lambda\|\underbrace{\mathbf{\Psi x}}_{\mathbf{s}}\|_1$$

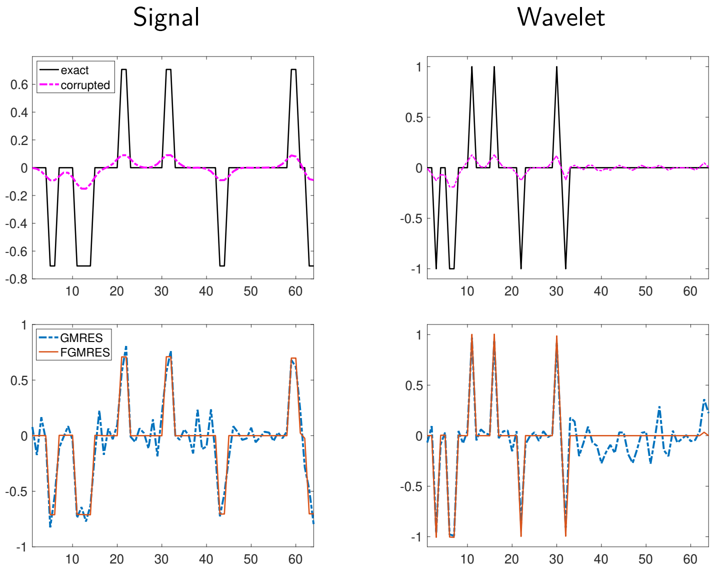
Solution subspace for flexible Arnoldi:

$$\mathbf{s}_k \in \operatorname{span}\{\mathbf{L}_1^{-1}\widehat{\mathbf{v}}_1, \mathbf{L}_2^{-1}\widehat{\mathbf{v}}_2, \dots, \mathbf{L}_k^{-1}\widehat{\mathbf{v}}_k\}, \quad \text{where} \quad \begin{array}{rcl} \widehat{\mathbf{v}}_1 & = & \mathbf{d}/\|\mathbf{d}\|_2 \\ \widehat{\mathbf{v}}_2 & = & \mathrm{ONC}(\mathbf{HL}_1^{-1}\widehat{\mathbf{v}}_1) \\ \widehat{\mathbf{v}}_3 & = & \mathrm{ONC}(\mathbf{HL}_2^{-1}\widehat{\mathbf{v}}_2) \\ \dots & & \end{array}$$

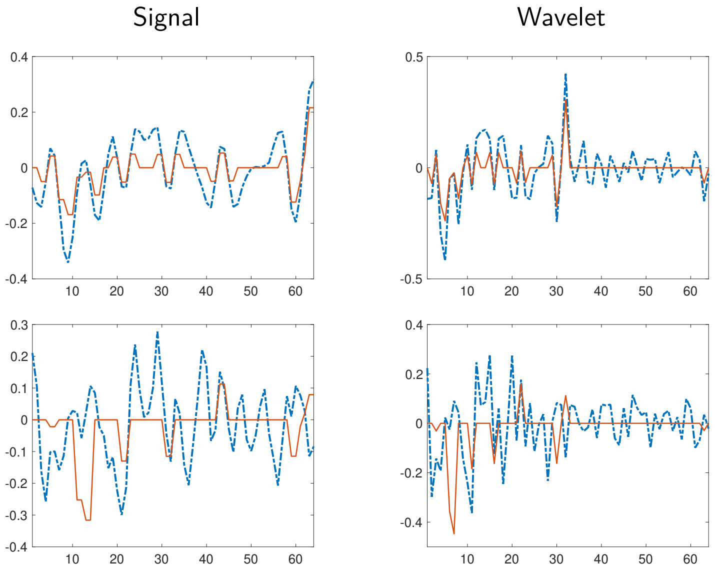
$$\mathbf{x}_k = \mathbf{\Psi}^{-1}\mathbf{s}_k$$

Analogously for flexible Golub-Kahan (possibly without $\widetilde{\mathbf{\Psi}}$).

An illustration: sparsity in a wavelet domain



An illustration: 2^{nd} and 4^{th} basis vectors



TV penalization

Let $\mathcal{R}(\mathbf{x}) = \mathrm{TV}(\mathbf{x})$.

- 1d case:
  $\mathrm{TV}(\mathbf{x}) = \|\mathbf{D}_{1\mathrm{d}}\mathbf{x}\|_1 \simeq \|\mathbf{W}_{1\mathrm{d}}\mathbf{D}\mathbf{x}\|_2^2$, where

$$\mathbf{D}_{1\mathrm{d}} = \begin{bmatrix} 1 & -1 & & \\ & \ddots & \ddots & \\ & & 1 & -1 \end{bmatrix} \in \mathbb{R}^{(N-1)\times N}, \quad \mathbf{W} = \mathrm{diag}\left(|\mathbf{D}_{1\mathrm{d}}\mathbf{x}|^{-1/2}\right)$$

- 2d case:
  [Wohlberg and Rodriguez. An iteratively reweighted norm algorithm for TV. *IEEE*, 2007]
  $\mathrm{TV}(\mathbf{x}) = \|\left((\mathbf{D}^{\mathrm{h}}\mathbf{x})^2 + (\mathbf{D}^{\mathrm{v}}\mathbf{x})^2\right)^{1/2}\|_1 \simeq \|\mathbf{W}\mathbf{D}_{2\mathrm{d}}\mathbf{x}\|_2^2$, where

$$\mathbf{D}_{2\mathrm{d}} = \begin{bmatrix} \mathbf{D}^{\mathrm{h}} \\ \mathbf{D}^{\mathrm{v}} \end{bmatrix} = \begin{bmatrix} \mathbf{D}_{1\mathrm{d}} \otimes \mathbf{I} \\ \mathbf{I} \otimes \mathbf{D}_{1\mathrm{d}} \end{bmatrix}, \hat{\mathbf{W}} = \mathrm{diag}\left(\left((\mathbf{D}^{\mathrm{h}}\mathbf{x})^2 + (\mathbf{D}^{\mathrm{v}}\mathbf{x})^2\right)^{-1/4}\right), W = \begin{bmatrix} \hat{\mathbf{W}} & 0 \\ 0 & \hat{\mathbf{W}} \end{bmatrix}$$

Smoothing Norm, $\mathbf{A} \in \mathbb{R}^{N\times N}$

Standard form transformation:

$$\bar{\mathbf{y}}_L = \arg\min_{\bar{\mathbf{y}}} \|\bar{\mathbf{A}}\bar{\mathbf{y}} - \bar{\mathbf{b}}\|_2^2 + \lambda\|\bar{\mathbf{y}}\|_2^2 \,, \quad \text{where} \quad \begin{array}{rcl} \bar{\mathbf{A}} & = & \mathbf{A}\mathbf{L}_{\mathbf{A}}^{\dagger} = \mathbf{A}[\mathbf{I} - (\mathbf{A}(\mathbf{I} - \mathbf{L}^{\dagger}\mathbf{L}))^{\dagger}\mathbf{A}] \\ \bar{\mathbf{b}} & = & \mathbf{b} - \mathbf{A}\mathbf{x}_0 \\ \mathbf{x}_L & = & \mathbf{L}_A^{\dagger}\bar{\mathbf{y}}_L + x_0 = \bar{\mathbf{x}}_L + \mathbf{x}_0 \end{array} .$$

Smoothing Norm, $\mathbf{A} \in \mathbb{R}^{N\times N}$

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[Hansen and Jensen. Smoothing-Norm Preconditioning for Reg. Min.-Res. *SIMAX*, 2007]

Write:

$$\mathbf{x}_L = \bar{\mathbf{x}}_L + \mathbf{x}_0 = \mathbf{L}_A^{\dagger}\bar{\mathbf{y}}_L + \mathbf{x}_0 = \mathbf{L}_A^{\dagger}\bar{\mathbf{y}}_L + \mathbf{K}\mathbf{t}_0\,, \quad \text{where} \quad \mathcal{R}(\mathbf{K}) = \mathcal{N}(\mathbf{L})\,, \quad \mathbf{L}_A^{\dagger} \text{ rectangular}\,.$$

Equivalently:

$$\mathbf{A}\left[\mathbf{L}_A^{\dagger},\ \mathbf{K}\right]\begin{bmatrix} \bar{\mathbf{y}}_L \\ \mathbf{t}_0 \end{bmatrix} = \mathbf{b}\,,$$

and, further:

$$\begin{bmatrix} (\mathbf{L}_A^{\dagger})^T\mathbf{A}\mathbf{L}_A^{\dagger} & (\mathbf{L}_A^{\dagger})^T\mathbf{A}\mathbf{K} \\ \mathbf{K}^T\mathbf{A}\mathbf{L}_A^{\dagger} & \mathbf{K}^T\mathbf{A}\mathbf{K} \end{bmatrix}\begin{bmatrix} \bar{\mathbf{y}}_L \\ \mathbf{t}_0 \end{bmatrix} = \begin{bmatrix} (\mathbf{L}_A^{\dagger})^T\mathbf{b} \\ \mathbf{K}^T\mathbf{b} \end{bmatrix}.$$

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Standard form transformation:

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$$\begin{bmatrix} (\mathbf{L}_A^{\dagger})^T\mathbf{A}\mathbf{L}_A^{\dagger} & (\mathbf{L}_A^{\dagger})^T\mathbf{A}\mathbf{K} \\ \mathbf{K}^T\mathbf{A}\mathbf{L}_A^{\dagger} & \mathbf{K}^T\mathbf{A}\mathbf{K} \end{bmatrix}\begin{bmatrix} \bar{\mathbf{y}}_L \\ \mathbf{t}_0 \end{bmatrix} = \begin{bmatrix} (\mathbf{L}_A^{\dagger})^T\mathbf{b} \\ \mathbf{K}^T\mathbf{b} \end{bmatrix}.$$

Schur complement system:

$$(\mathbf{L}_A^{\dagger})^T\mathbf{P}\mathbf{A}\mathbf{L}_A^{\dagger}\bar{\mathbf{y}} = (\mathbf{L}_A^{\dagger})^T\mathbf{P}\mathbf{b}, \quad \text{where} \quad \mathbf{P} = \mathbf{I} - \mathbf{A}\mathbf{K}(\mathbf{K}^T\mathbf{A}\mathbf{K})^{-1}\mathbf{K}^T \in \mathbb{R}^{N\times N}.$$

TV regularization, $\mathbf{A} \in \mathbb{R}^{N \times N}$

[G. and Sabaté Landman (2019)]

Similar idea, with reweighting...

$$(\mathbf{D}^{\dagger})^T \mathbf{P}\mathbf{A}(\mathbf{W}\mathbf{D})_A^{\dagger}\bar{\mathbf{y}} = (\mathbf{D}^{\dagger})^T \mathbf{P}\mathbf{b}$$

Building a better approximation subspace for the solution!

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Building a better approximation subspace for the solution!

- $\mathbf{L} = \mathbf{W}\mathbf{D}$ (with $\mathbf{W} = \mathbf{W}(\mathbf{x}_k)$):
  flexible GMRES (instead of restarted GMRES);

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[G. and Sabaté Landman (2019)]

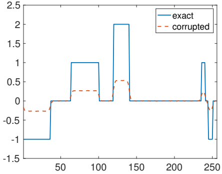
Similar idea, with reweighting...

$$(\mathbf{D}^{\dagger})^T \mathbf{P} \mathbf{A} (\mathbf{W}\mathbf{D})^{\dagger}_{A} \bar{\mathbf{y}} = (\mathbf{D}^{\dagger})^T \mathbf{P} \mathbf{b}$$

Building a better approximation subspace for the solution!

- $\mathbf{L} = \mathbf{W}\mathbf{D}$ (with $\mathbf{W} = \mathbf{W}(\mathbf{x}_k)$):
  flexible GMRES (instead of restarted GMRES);
- large-scale computations:
  - approximating $\mathbf{L}^{\dagger}$
    (exploiting structure, and running preconditioned LSQR or LSMR)
  - thresholding the weights

A simple 1D example...



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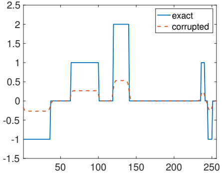
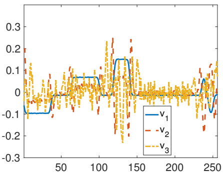
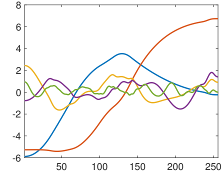
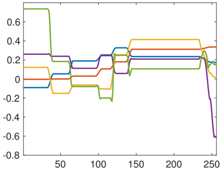
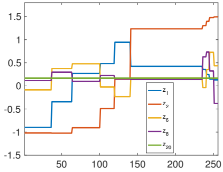


basis vectors









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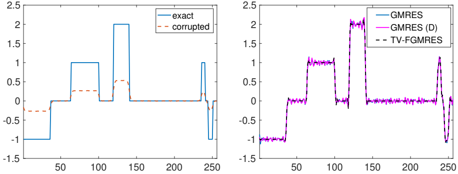


basis vectors

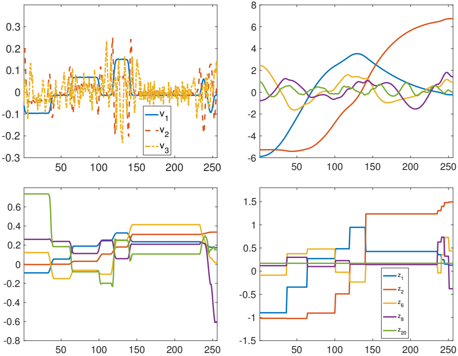


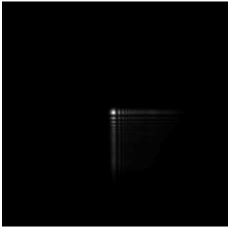
Image deblurring example with $\mathbf{\Psi} = \mathbf{I}$

[G., Hansen, Nagy. *IR Tools* (2018)]
https://github.com/silviagazzola/IRtools

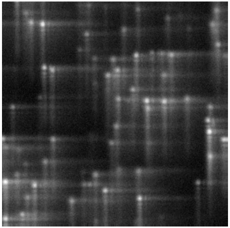
http://www2.compute.dtu.dk/ pcha/IRtools/

true

PSF

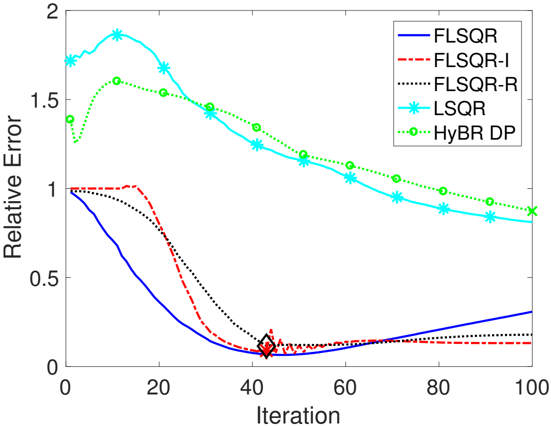


observed



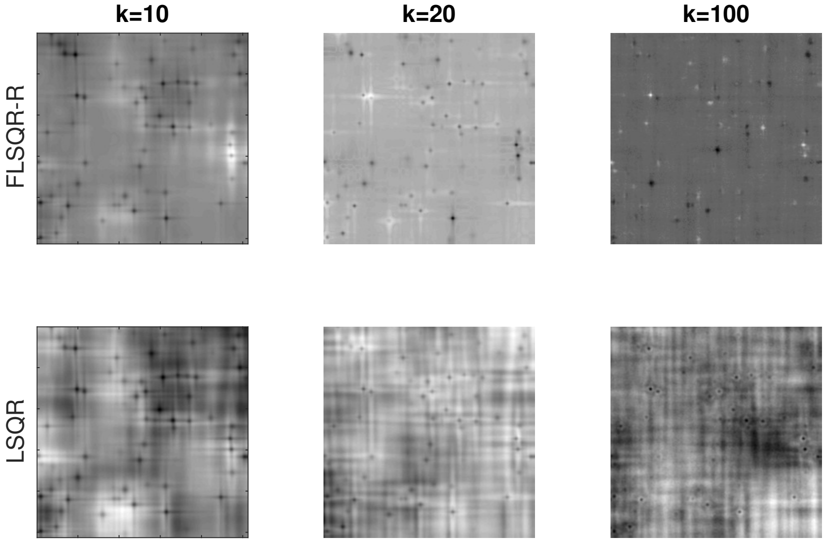
- Image is 256×256 pixels
- Noise level is 5×10^{-2}
- Reflexive boundary conditions

Reconstruction errors

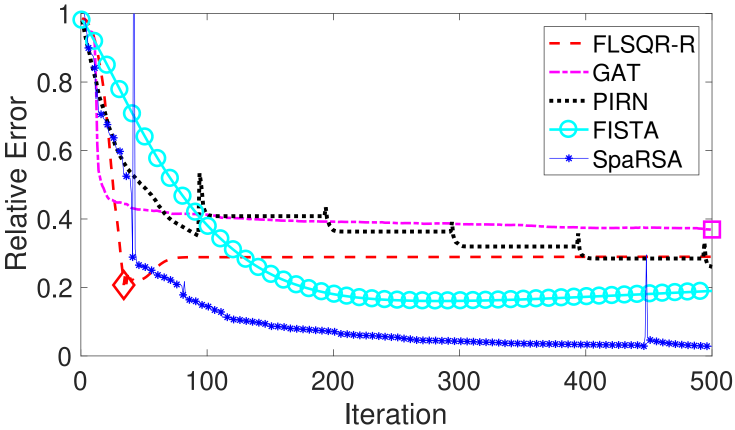


- Reconstruction errors computed as $\frac{\|\mathbf{x}_k - \mathbf{x}_{\text{true}}\|_2}{\|\mathbf{x}_{\text{true}}\|_2}$
- λ for FLSQR-I and FLSQR-R use discrepancy principle

Basis images



Comparison to other methods



- GAT = Generalized Arnoldi-Tikhonov
- PIRN† = Preconditioned iteratively re-weighted norm
- FISTA† = Fast iterative-shrinkage-thresholding algorithm
- SpaRSA† = Sparse Reconstruction by Separable Approximation

(† uses λ from FLSQR-R)

Tomography example with $\mathbf{\Phi} \neq \mathbf{I}$

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[G., Hansen, Nagy. *IR Tools* (2018)]

```
n = 256; optn = PRtomo('defaults');
optn=PRset(optn,'angles',0:2:179,'p',round(sqrt(2)*n),'d',sqrt(2)*n);
[A, b, x, ProbInfo] = PRtomo(n, optn);
```

- phantom is 256×256 pixels
- $\mathbf{A}$ has size 32580×65536 (approx. 50% undersampling)

Tomography example with $\mathbf{\Phi} \neq \mathbf{I}$

[G., Hansen, Nagy. *IR Tools* (2018)]

```
n = 256; optn = PRtomo('defaults');
optn=PRset(optn,'angles',0:2:179,'p',round(sqrt(2)*n),'d',sqrt(2)*n);
[A, b, x, ProbInfo] = PRtomo(n, optn);
figure, PRshowx(x, ProbInfo)
```

- phantom is 256×256 pixels
- $\mathbf{A}$ has size 32580×65536 (approx. 50% undersampling)

Tomography example with $\mathbf{\Phi} \neq \mathbf{I}$

[G., Hansen, Nagy. *IR Tools* (2018)]

```
n = 256; optn = PRtomo('defaults');
optn=PRset(optn,'angles',0:2:179,'p',round(sqrt(2)*n),'d',sqrt(2)*n);
[A, b, x, ProbInfo] = PRtomo(n, optn);
figure, PRshowx(x, ProbInfo)
bn = PRnoise(b, 1e-2);
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- $\mathbf{\Psi}$ is a 4-level 2D Haar wavelet transform

Reconstructed phantoms

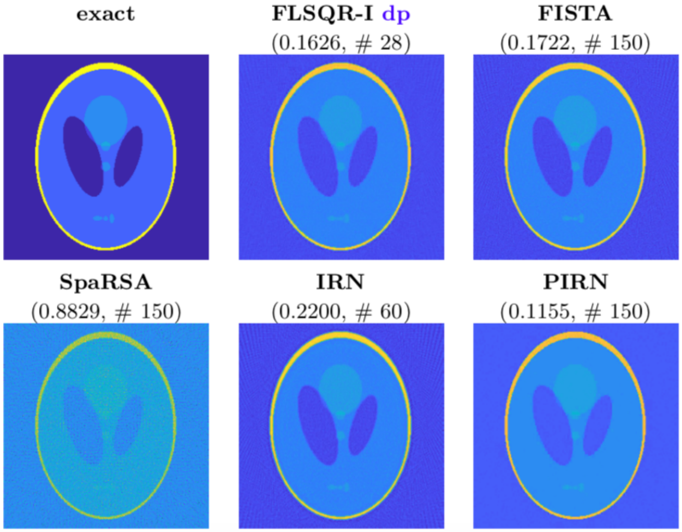


Image deblurring example

[G., Hansen, Nagy. *IR Tools* (2018)]

Cameraman example: 256×256 pixels.

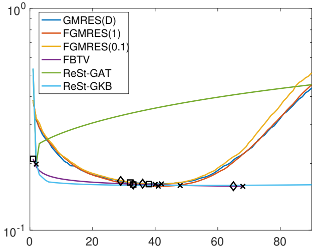
blurred & noisy

SN-GMRES

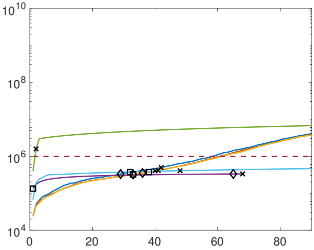
TV-FGMRES

fast gradient-based method

Image deblurring example



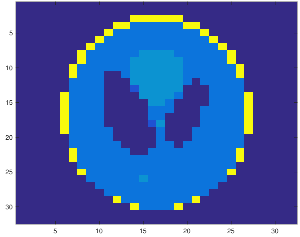
Relative Error History

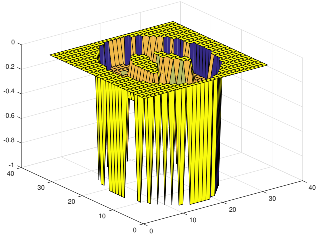


Total Variation History

Tomography example with flexible TV regularization

small PRtomo example: 32×32 pixels; $\mathbf{A} \in \mathbb{R}^{2025\times 1024}$
... ongoing work





Exact phantom
noisy (Gaussian white noise, $\|\mathbf{e}\|/\|\mathbf{b}^{\mathrm{true}}\| = 10^{-2}$) image

Tomography example with flexible TV regularization

small `PRtomo` example: 32×32 pixels; $\mathbf{A} \in \mathbb{R}^{2025 \times 1024}$

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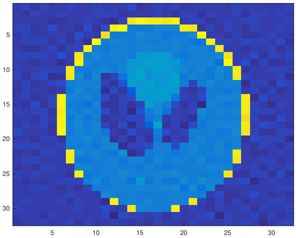
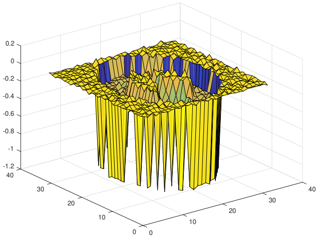
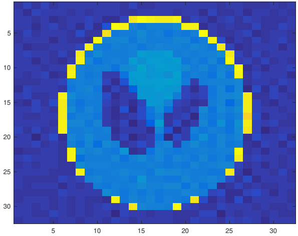


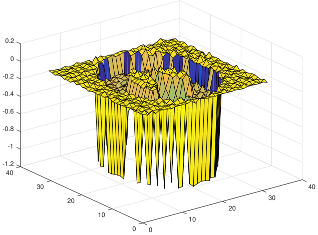


LSQR

Tomography example with flexible TV regularization

small PRtomo example: 32×32 pixels; $\mathbf{A} \in \mathbb{R}^{2025 \times 1024}$
... ongoing work

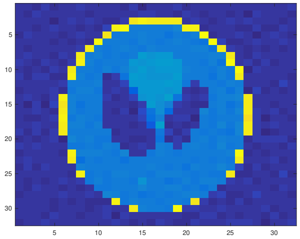


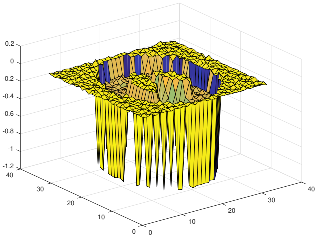


LSQR (D)

Tomography example with flexible TV regularization

small PRtomo example: 32×32 pixels; $\mathbf{A} \in \mathbb{R}^{2025 \times 1024}$
... ongoing work



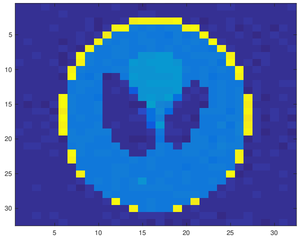


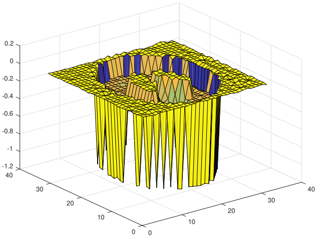
TV-LSQR

Tomography example with flexible TV regularization

small PRtomo example: 32×32 pixels; $\mathbf{A} \in \mathbb{R}^{2025 \times 1024}$

... ongoing work





TV-LSQR "0 norm"

Summary of benefits ...

- **Flexible Krylov methods**
  - ✔ Avoid inner-outer schemes (current solution immediately incorporated in basis)
  - ✔ Both square (flexible Arnoldi) non-square problems (flexible Golub-Kahan)
  - ✔ Optimality and equivalency results
- **Hybrid method**
  - ✔ Stabilize reconstruction errors
  - ✔ Automatic choice of λ and stopping criteria
- **Transformed problem**
  - ✔ Enforce sparsity in a transform
  - ✔ Connections to multi-parameter regularization

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References

- J. Chung and S. G. *Flexible Krylov methods for ℓ^p regularization*. SISC, 2019.
- S. G. and M. Sabaté Landman. *Flexible GMRES for Total Variation regularization*. BIT, 2019.
- S. G., P. C. Hansen, and J. Nagy. *IR Tools: A MATLAB Package of Iterative Regularization Methods and Large-Scale Test Problems*. Numer. Algorithms, 2018. https://github.com/silviagazzola/IRtools