

Fast Nonnegative Least Squares through flexible Krylov subspaces

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What is this talk about?

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Solution of

$$\min_{x \in \mathbb{R}^N} \|b - Ax\|_2, \quad A \in \mathbb{R}^{N \times N}, \quad b \in \mathbb{R}^N,$$

coming from suitable discretization of

$$\int_{\Omega} k(s, t) f(t) dt = g(s).$$

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Modeling inverse problems:

- the process k , the output g ($g = g^{\text{ex}} + \varepsilon$) are known;
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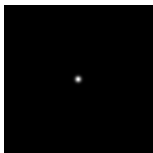
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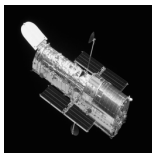
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An example: **image deblurring and denoising**.



PSF

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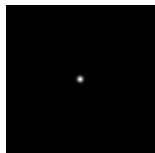
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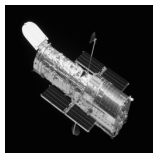
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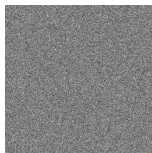
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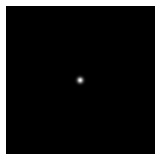
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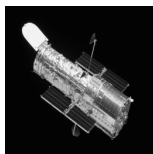
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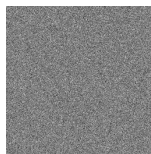
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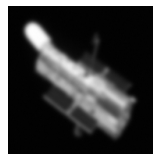
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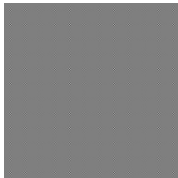
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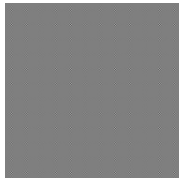
available

$$x = A^\dagger b$$



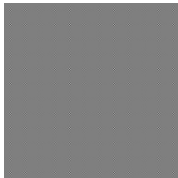
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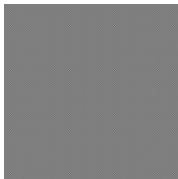


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Nonnegative constraints!

$$\min_{x \geq 0} \|b - Ax\|_2$$



Outline

1 Nonnegative LS problems

- Brief survey of the available methods
- Krylov methods for unconstrained problems

2 Flexible Krylov subspaces

- The need of introducing “flexibility”
- Deriving FCGLS
- MFCGLS for nonnegative LS problems

3 Numerical Experiments

- Restoration of Astronomical Images
- CT Reconstruction

4 Looking at Poisson noise

- Modeling Poisson Noise
- CP-MFCGLS

5 Final Remarks

Popular approaches

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■ Projected gradient

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$$x_{m+1} = P_+(x_m + \alpha_m A^T(b - Ax_m)).$$

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[Beck and Teboulle. [FISTA](#), *SIIMS*, 2009]

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■ Active set methods

[Morigi, Plemmons, Reichel, Sgallari. Hybrid multilevel-active set method for box-constr. *Calcolo*, 2011]

Krylov methods for unconstrained problems

Unconstrained LS problem:

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Iterative methods such that:

- $x_m \in \mathcal{K}_m(C, d)$, where

$$\mathcal{K}_m(C, d) = \text{span}\{d, Cd, \dots, C^{m-1}d\},$$

and $C = A, A^T A, AA^T, d = b, A^T b, A^\ell b (\ell \geq 1)$.

- $r_m := b - Ax_m$ satisfies some conditions, e.g.,

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Extremely efficient!

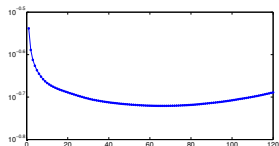
Reichel & CO., Hansen & CO., Nagy & CO., Strakos & CO., Novati & CO [...]

Lewis, Sgallari, Morigi, Lanza, Calvetti, Hanke, Donatelli, Chung, Elden, Simoncini, Jensen, Rodriguez, Russo, O'Leary,

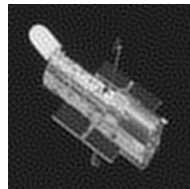
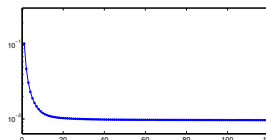
Plemmons, Jorgensen, Kilmer, Hnetynkova, Hochstenbach, Noschese, Dykes, Hayami, Ye, Saunders, Palmer, Huang, Jia [...]

Krylov methods (CGLS) in action

relative errors

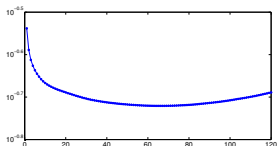


relative residuals

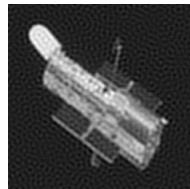
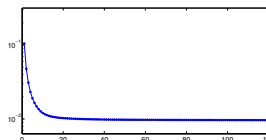


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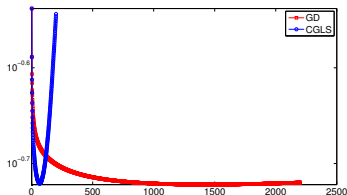


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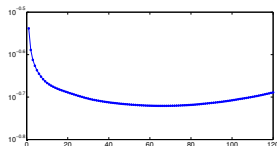
Gradient Descent approach VS. Krylov Subspaces approach

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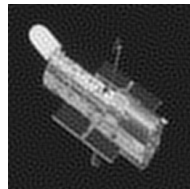
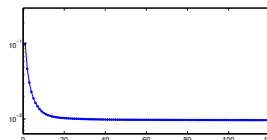


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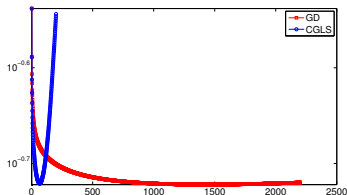


relative residuals



Gradient Descent approach VS. Krylov Subspaces approach

relative errors



They work efficiently as:

- they mimic the TSVD;
- $\mathcal{K}_m(C, d) \simeq \mathcal{K}_{m+1}(C, d)$ for small m .

Defining Krylov methods

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Explicitly computing the solution along descent directions:

$$x_{m+1} = x_m + \sum_{j=0}^m \alpha_j^{(m)} d_j$$

$$d_{m+1} = \bar{z}_{m+1} + \sum_{j=0}^m \beta_j^{(m)} d_j .$$

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Requiring Ad_j orthogonal and minimal residual:

- $x_{m+1} = x_m + \alpha_m d_m$, where $\alpha_m = \frac{(r_m, Ad_m)}{(Ad_m, Ad_m)}$;
- $\beta_j^{(m)} = -\frac{(A\bar{z}_{m+1}, Ad_j)}{(Ad_j, Ad_j)}$, $j = 0, \dots, m$.

Special case: **CGLS**.

The need of introducing “flexibility”

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Back the KKT conditions, most general case:

$$XA^T(b - Ax_m) = 0, \quad x_m \geq 0$$

- make sure that $x_m \geq 0$ for each m .

The need of introducing “flexibility”

Back the KKT conditions, most general case:

$$X^{(m)} A^T (b - A x_m) = 0, \quad x_m \geq 0$$

where, at the m th step, $X^{(m)} = \text{diag}(x_{m-1})$.

- variable “preconditioners”;
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We need a Krylov method (CGLS) that handles:

- variable “preconditioners”;
- make sure that $x_m \geq 0$ for each m .

[Simoncini and Szyld. Recent computational developments in Krylov meth, *NLAA*, 2007]

Flexible Krylov methods for regularization

“Preconditioners” that enforce “regularity”

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$$\blacksquare \min_{x \in \mathbb{R}^N} \|b - Ax\|_2^2 + \lambda \|x\|_1 \quad \equiv \quad \min_{x \in \mathbb{R}^N} \|b - AX^{(m)}x\|_2^2 + \lambda \|x\|_2^2$$

[G. and Nagy. GAT for sparse reconstruction. SISC, 2014]

$$\blacksquare \min_{x \in \mathbb{R}^N} \|b - Ax\|_2^2 \quad \longrightarrow \quad x_m = Z_m y_m$$

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[Reichel, Yu. Tikhonov regularization via flexible Arnoldi. BIT, 2015]

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now... deriving **FCGLS**

If no preconditioners: CGLS

Input: A , b , x_0 .

Initialize: $r_0 = b - Ax_0$, $\bar{z}_0 = A^T r_0$.

Take $d_0 = \bar{z}_0$.

For $m = 0, \dots$, till a stopping criterion is satisfied

- Set $\alpha_m = \frac{(r_m, Ad_m)}{(Ad_m, Ad_m)}$.
 - Update $x_{m+1} = x_m + \alpha_m d_m$.
 - Update $r_{m+1} = r_m - \alpha_m Ad_m$.
 - Compute $\bar{z}_{m+1} = A^T r_{m+1}$.
-
- Set $\beta_m = -\frac{(A\bar{z}_{m+1}, Ad_m)}{(Ad_m, Ad_m)}$.
 - Update $d_{m+1} = \bar{z}_{m+1} + \beta_m d_m$.

If the preconditioner L is fixed: PCGLS

Input: A , L , b , x_0 .

Initialize: $r_0 = b - Ax_0$, $z_0 = A^T r_0$.

Compute $\bar{z}_0 = Lz_0$.

Take $d_0 = \bar{z}_0$.

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- Update $d_{m+1} = \bar{z}_{m+1} + \beta_m d_m$.

If the “preconditioners” $L^{(m)}$ are variable: FCGLS

Input: A , $L^{(0)}$, b , x_0 .

Initialize: $r_0 = b - Ax_0$, $z_0 = A^T r_0$.

Compute $\bar{z}_0 = L^{(0)} z_0$.

Take $d_0 = \bar{z}_0$.

For $m = 0, \dots$, till a stopping criterion is satisfied

- Set $\alpha_m = \frac{(r_m, Ad_m)}{(Ad_m, Ad_m)}$.
- Update $x_{m+1} = x_m + \alpha_m d_m$.
- Update $r_{m+1} = r_m - \alpha_m Ad_m$.
- Compute $z_{m+1} = A^T r_{m+1}$.
- Compute $L^{(m+1)}$.
- Compute $\bar{z}_{m+1} = L^{(m+1)} z_{m+1}$.
- Set $\beta_j^{(m)} = -\frac{(A\bar{z}_{m+1}, Ad_j)}{(Ad_j, Ad_j)}$, $j = 0, \dots, m$.
- Update $d_{m+1} = \bar{z}_{m+1} + \sum_{j=0}^m \beta_j^{(m)} d_j$.

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- Update $d_{m+1} = \bar{z}_{m+1} + \sum_{j=\hat{m}}^m \beta_j^{(m)} d_j$.

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Solving:

$$X^{(m)} A^T (b - Ax) = 0, \quad x \geq 0, \quad \text{with} \quad X^{(m)} = \text{diag}(x_m),$$

by FCGLS:

$$x_{m+1} = x_m + \alpha_m d_m.$$

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Solving:

$$X^{(m)} A^T (b - Ax) = 0, \quad x \geq 0, \quad \text{with} \quad X^{(m)} = \text{diag}(x_m),$$

by **FCGLS**:

$$x_{m+1} = x_m + \alpha_m d_m.$$

To guarantee nonnegativity at each step:

$$\alpha_m = \min \left(\alpha_m, \min \left(-\frac{x_m(d_m < 0)}{d_m(d_m < 0)} \right) \right).$$

MFCGLS for nonnegative LS problems

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Prone to stagnation: $\alpha_m = 0$!!!

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MFCGLS (Modified FCGLS)

Input: A , b , $x_0^0 \geq 0$.

- For $k = 0, \dots$, till a stopping criterion is satisfied
 - For $m = 0, \dots$, till m_{\max} or $\alpha_m = 0$
 - Run a **FCGLS** with initial guess x_0^k , preconditioner $X^{(m)}$, and NN:

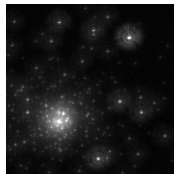
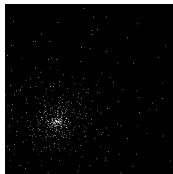
$$x_{m+1} = x_m + \alpha_m d_m;$$

$$d_{m+1} = \bar{z}_{m+1} + \sum_{j=\hat{m}}^m \beta_j^{(m)} d_j.$$
 - Restart with the last approximation.

Numerical experiments

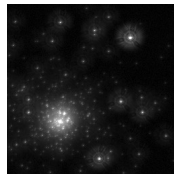
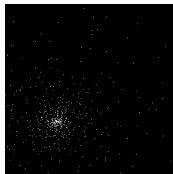
Numerical experiments

■ star_cluster test problem [Nagy et al. *Restore Tools*, 2012]

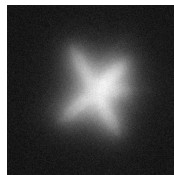
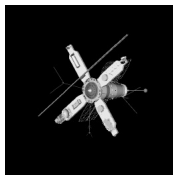


Numerical experiments

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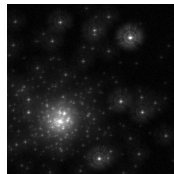
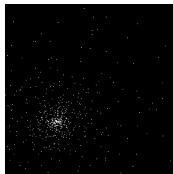


■ satellite test problem [Nagy et al. *Restore Tools*, 2012]

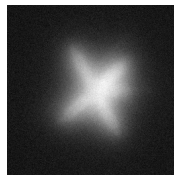
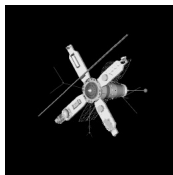


Numerical experiments

■ star_cluster test problem [Nagy et al. *Restore Tools*, 2012]



■ satellite test problem [Nagy et al. *Restore Tools*, 2012]



■ paralleltomo test problem [Hansen et al. *AIR Tools*, 2012]

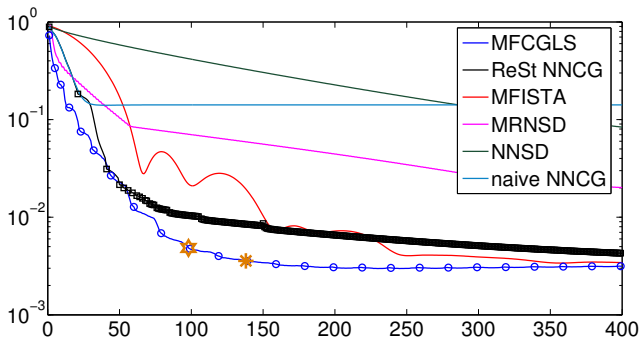
star_cluster test problem

$$A \in \mathbb{R}^{65536 \times 65536}, \tilde{\varepsilon} = 10^{-2}$$

star_cluster test problem

$$A \in \mathbb{R}^{65536 \times 65536}, \tilde{\varepsilon} = 10^{-2}$$

Relative Error History



ReSt NNCG by

[Calvetti et al. Non-neg. and iterative methods for ill-posed pb, *Inv. Problems*, 2004]

star_cluster test problem

$$A \in \mathbb{R}^{65536 \times 65536}, \tilde{\varepsilon} = 10^{-2}$$

	rel.error	iterations	tot.time	av.time
MFCGLS	2.8132e-03	248.67	62.56	0.25
ReSt NNCG	5.3699e-03	261.00	113.51	0.43
FISTA	9.1283e-02	72.00	42.06	0.58
MFISTA	3.2803e-03	400.00	216.11	0.54
MFISTA(0.2)	3.2445e-03	400.00	194.78	0.49
MFISTA(5)	4.2834e-03	400.00	185.22	0.46
MRNSD	1.9889e-02	400.00	91.11	0.23
NNSD	8.3206e-02	400.00	91.59	0.23
naive NNCG	1.4028e-01	400.00	105.02	0.26

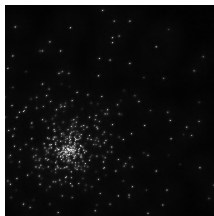
star_cluster test problem

$A \in \mathbb{R}^{65536 \times 65536}$, $\tilde{\varepsilon} = 10^{-2}$, 200th iteration

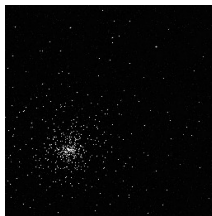
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$A \in \mathbb{R}^{65536 \times 65536}$, $\tilde{\varepsilon} = 10^{-2}$, 200th iteration

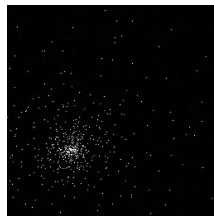
MRNSD



ReSt NNCG



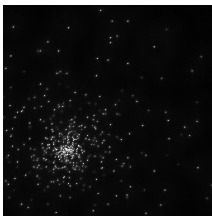
MFCGLS



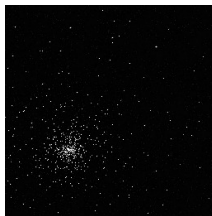
star_cluster test problem

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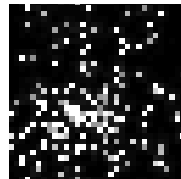
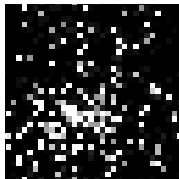
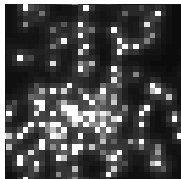
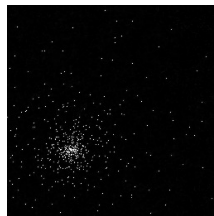
MRNSD



ReSt NNCG



MFCGLS

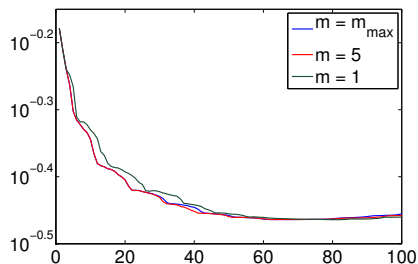
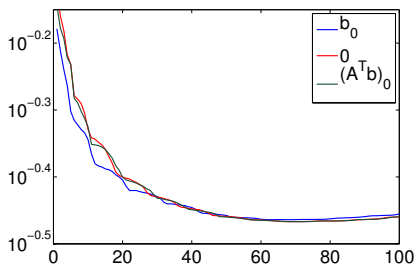


satellite test problem

satellite test problem

$$A \in \mathbb{R}^{65536 \times 65536}, \tilde{\varepsilon} = 10^{-1}$$

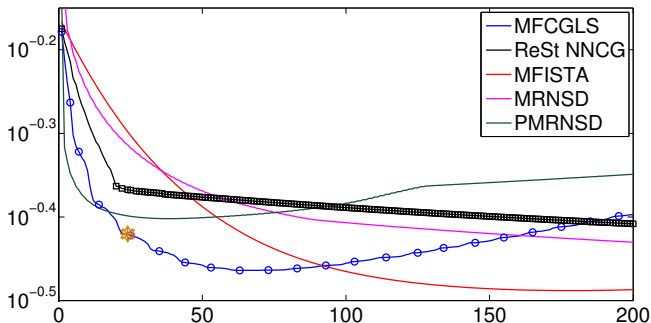
Relative Error Histories, varying some “side” parameters



satellite test problem

$$A \in \mathbb{R}^{65536 \times 65536}, \tilde{\varepsilon} = 10^{-1}$$

Relative Error History



ReSt NNCG by

[Hanke, Nagy, and Plemmons. Preconditioned iterative regularization, *Num.Lin.Alg.*, 1993]

satellite test problem

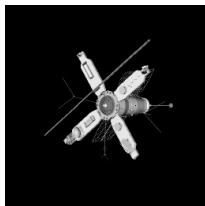
$$A \in \mathbb{R}^{65536 \times 65536}, \tilde{\varepsilon} = 10^{-1}$$

	rel.error	iterations	tot.time	av.time
MFCGLS	3.5098e-01	70.33	5.49	0.08
ReSt NNCG	4.0957e-01	106.67	9.38	0.08
FISTA	3.2969e-01	164.33	21.22	0.12
MFISTA	3.2583e-01	177.00	23.10	0.13
MFISTA(0.2)	3.3318e-01	137.00	20.58	0.15
MFISTA(5)	3.3397e-01	200.00	26.86	0.13
MRNSD	3.7720e-01	200.00	12.55	0.06
PMRNSD	4.0032e-01	37.33	2.62	0.07
NNSD	4.3095e-01	200.00	13.82	0.07

satellite test problem

$$A \in \mathbb{R}^{65536 \times 65536}, \tilde{\varepsilon} = 10^{-1}$$

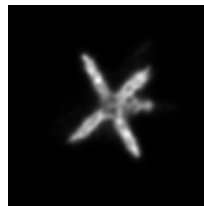
exact



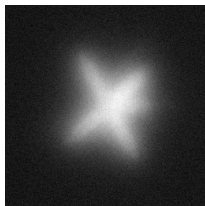
MFCGLS (# 84)



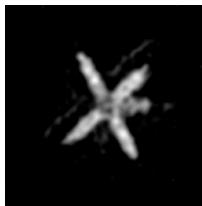
MRNSD (# 200)



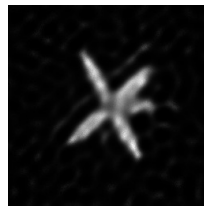
blurred & noisy



MFISTA (# 200)



PMRNSD (# 30)



parallel tomo test problem

parallel tomo test problem

overdetermined (81088×65536 coefficient matrix, $\tilde{\varepsilon} = 5 \cdot 10^{-2}$)

	rel.error	iterations	tot.time	av.time
MFCGLS	1.8268e-01	17.33	0.92	0.09
ReSt NNCG	2.0133e-01	56.00	16.31	0.11
MFISTA	2.0029e-01	37.00	53.13	1.44
MRNSD	1.8506e-01	45.00	4.10	0.09
Cimmino	1.9982e-01	100.00	33.47	0.33

parallel tomo test problem

overdetermined (81088×65536 coefficient matrix, $\tilde{\varepsilon} = 5 \cdot 10^{-2}$)

	rel.error	iterations	tot.time	av.time
MFCGLS	1.8268e-01	17.33	0.92	0.09
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MFISTA	2.0029e-01	37.00	53.13	1.44
MRNSD	1.8506e-01	45.00	4.10	0.09
Cimmino	1.9982e-01	100.00	33.47	0.33

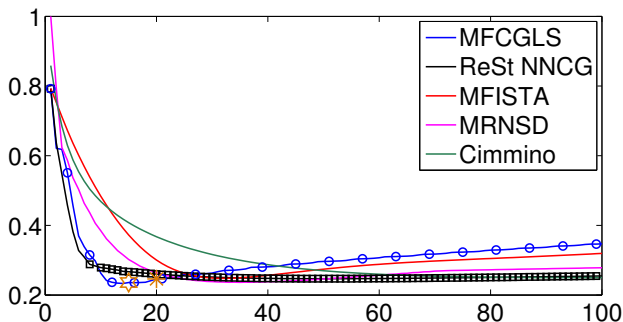
underdetermined (32580×65536 coefficient matrix, $\tilde{\varepsilon} = 5 \cdot 10^{-2}$)

	rel.error	iterations	tot.time	av.time
MFCGLS	2.3145e-01	13.00	0.15	0.07
ReSt NNCG	2.4572e-01	51.00	0.59	0.05
MFISTA	2.4634e-01	32.00	12.41	0.39
MRNSD	2.3485e-01	35.00	3.43	0.09
Cimmino	2.4715e-01	94.33	8.84	0.09

underdetermined parallel tomo test problem

$$A \in \mathbb{R}^{65160 \times 65536}, \tilde{\varepsilon} = 5 \cdot 10^{-2}.$$

Relative Error History



underdetermined parallel tomo test problem

$A \in \mathbb{R}^{65160 \times 65536}$, $\tilde{\varepsilon} = 5 \cdot 10^{-2}$, 17th iteration

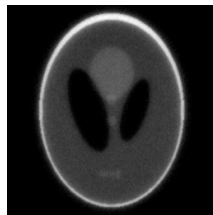
exact



MFCGLS



MFISTA



Incorporating Poisson noise

$$b = \text{Poisson}(Ax^{\text{ex}}) + \text{Poisson}(\beta \mathbf{1}) + \text{Normal}(0, \sigma^2 I)$$

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[Snyder et al.. Image recovery from CCD, *J. Opt. Soc. Amer. A*, 1993]

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[Snyder et al.. Image recovery from CCD, *J. Opt. Soc. Amer. A*, 1993]

$$\underbrace{b - \beta \mathbf{1}}_{=: b_\beta} = Ax^{\text{ex}} + \underbrace{\text{Normal}(0, \text{diag}(Ax^{\text{ex}} + \beta \mathbf{1} + \sigma^2 \mathbf{1}))}_{=: C_\eta}.$$

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[Bardsley and Nagy. Covariance-prec. meth. for NN, *SIMAX*, 2006]

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Problem to solve:

$$\min_{x \geq 0} \|C_\eta^{-1/2}(b_\beta - Ax)\|_2^2,$$

by the class of MRNSD methods:

Incorporating Poisson noise

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Problem to solve:

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► **WMRNSD** : $C_\eta = \text{diag}(b + \sigma^2 \mathbf{1});$

Incorporating Poisson noise

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[Snyder et al.. Image recovery from CCD, *J. Opt. Soc. Amer. A*, 1993]

[Bardsley and Nagy. Covariance-prec. meth. for NN, *SIMAX*, 2006]

$$\underbrace{b - \beta \mathbf{1}}_{=: b_\beta} = Ax^{\text{ex}} + \underbrace{\text{Normal}(0, \text{diag}(Ax^{\text{ex}} + \beta \mathbf{1} + \sigma^2 \mathbf{1}))}_{=: C_\eta}.$$

Problem to solve:

$$\min_{x \geq 0} \|C_\eta^{-1/2}(b_\beta - Ax)\|_2^2,$$

by the class of MRNSD methods:

- ▶ **WMRNSD** : $C_\eta = \text{diag}(b + \sigma^2 \mathbf{1});$
- ▶ $C_\eta^{(k)} = \text{diag}(Ax_k + \beta \mathbf{1} + \sigma^2 \mathbf{1}).$

Incorporating Poisson noise

$$b = \text{Poisson}(Ax^{\text{ex}}) + \text{Poisson}(\beta \mathbf{1}) + \text{Normal}(0, \sigma^2 I)$$

[Snyder et al.. Image recovery from CCD, *J. Opt. Soc. Amer. A*, 1993]

[Bardsley and Nagy. Covariance-prec. meth. for NN, *SIMAX*, 2006]

$$\underbrace{b - \beta \mathbf{1}}_{=: b_\beta} = Ax^{\text{ex}} + \underbrace{\text{Normal}(0, \text{diag}(Ax^{\text{ex}} + \beta \mathbf{1} + \sigma^2 \mathbf{1}))}_{=: C_\eta}.$$

Problem to solve:

$$\min_{x \geq 0} \|C_\eta^{-1/2}(b_\beta - Ax)\|_2^2,$$

by the class of MRNSD methods:

- ▶ WMRNSD : $C_\eta = \text{diag}(b + \sigma^2 \mathbf{1});$
- ▶ KWMRNSD : $C_\eta^{(k)} = \text{diag}(Ax_k + \beta \mathbf{1} + \sigma^2 \mathbf{1}).$

Introducing CP-MFCGLS

Input: A , b , $x_0^0 \geq 0$, $X^{(0)}$, $C_\eta^{(0)}$.

Initialize: $r_0^k = b - Ax_0^0$, $z_0^0 = A^T (C_\eta^{(0)})^{-1} r_0^0$, $\bar{z}_0^0 = X^{(0)} z_0^0$, $d_0^0 = \bar{z}_0^0$.

- For $k = 0, \dots$, till a stopping criterion is satisfied
 - For $m = 0, \dots$, till m_{\max} or $\alpha_m = 0$ or a stopping criterion is satisfied
 - Run a FCGLS with x_0^k , preconditioners $X^{(m)}$, $C_\eta^{(k)}$, and NN:
 - Compute $\alpha_m = \frac{(\bar{r}_m^k, (C_\eta^{(k)})^{-1/2} Ad_m^k)}{((C_\eta^{(k)})^{-1/2} Ad_m^k, (C_\eta^{(k)})^{-1/2} Ad_m^k)}$.
 - Update $x_{m+1}^k = x_m^k + \alpha_m d_m^k$.
 - Update $r_{m+1}^k = r_m^k - \alpha_m Ad_m^k$.
 - Compute $X^{(m+1)}$.
 - Compute $z_{m+1}^k = A^T (C_\eta^{(k)})^{-1} r_{m+1}^k$.
 - Compute $\bar{z}_{m+1}^k = X^{(m+1)} z_{m+1}^k$.
 - Set $\beta_j = -\frac{((C_\eta^{(k)})^{-1/2} Az_{m+1}^k, (C_\eta^{(k)})^{-1/2} Ad_m^k)}{((C_\eta^{(k)})^{-1/2} Ad_m^k, (C_\eta^{(k)})^{-1/2} Ad_m^k)}$, $j = \hat{m}, \dots, m$.
 - Update $d_{m+1}^k = \bar{z}_{m+1}^k + \sum_{j=\hat{m}}^m \beta_j d_j^k$.
 - Restart with the last approximation, and update $C_\eta^{(k+1)}$.

satellite test problem, Gaussian and Poisson noise

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$$A \in \mathbb{R}^{65536 \times 65536}$$

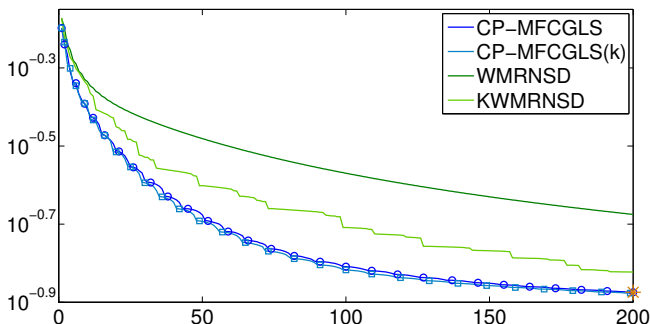
Gauss: $\sigma = 20$, Poisson: $\beta = 60$, $\tilde{\varepsilon} \simeq 1.5 \cdot 10^{-2}$

satellite test problem, Gaussian and Poisson noise

$$A \in \mathbb{R}^{65536 \times 65536}$$

Gauss: $\sigma = 20$, Poisson: $\beta = 60$, $\tilde{\varepsilon} \simeq 1.5 \cdot 10^{-2}$

Relative Error History



satellite test problem, Gaussian and Poisson noise

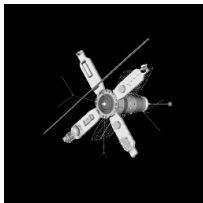
$$A \in \mathbb{R}^{65536 \times 65536}, \tilde{\varepsilon} \simeq 1.5 \cdot 10^{-2}$$

	rel.error	iterations	tot.time	av.time
CP-MFCGLS	1.2785e-01	300.00	31.65	0.08
CP-MFCGLS(<i>k</i>)	1.2778e-01	300.00	32.17	0.08
WMRNSD	1.8201e-01	300.00	28.34	0.09
KWMRNSD	1.3590e-01	300.00	37.19	0.12

satellite test problem, Gaussian and Poisson noise

$A \in \mathbb{R}^{65536 \times 65536}$, $\tilde{\varepsilon} \simeq 1.5 \cdot 10^{-2}$, 100th iteration

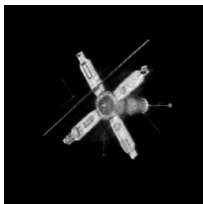
exact



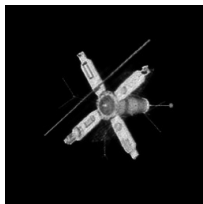
blurred & noisy



KWMRNSD



VP-MFCGLS



Final Remarks

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 - other Krylov methods (FGCR...);
 - ...

Paper available on arXiv:

S. Gazzola and Y. Wiaux.

Fast nonnegative least squares through flexible Krylov subspaces.

arXiv:1511.06269

Final Remarks

- Systematic and efficient way to enforce nonnegativity within Krylov subspace methods.
- Embraces and improves many methods already available.
- Possible generalizations:
 - box constraints;
 - sparsity (?);
 - other Krylov methods (FGCR...);
 - ...

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Thanks for your attention!