

Regularization by inexact Krylov methods with applications to blind deblurring

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Setting the stage: linear inverse problem

Solution of

$$\min_{x \in \mathbb{R}^n} \|Ax - b\|_2, \quad \text{where } Ax_{\text{true}} + e = b$$

and

$$b \in \mathbb{R}^m$$

available observations or measurements

$$x_{\text{true}} \in \mathbb{R}^n$$

unknown quantity of interest

$$A \in \mathbb{R}^{m \times n}$$

available ill-conditioned matrix models forward process

$$e \in \mathbb{R}^m$$

additive Gaussian white noise

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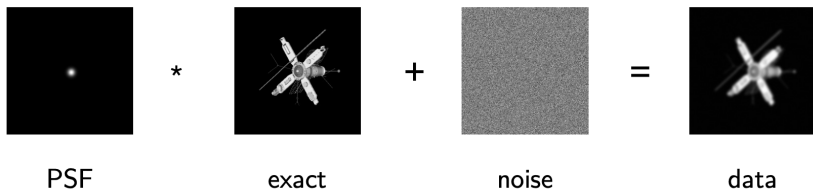
$$A \in \mathbb{R}^{m \times n}$$

available ill-conditioned matrix models forward process

$$e \in \mathbb{R}^m$$

additive Gaussian white noise

Example: [image deblurring](#)



Here $m = n = 65536$.

Setting the stage: separable nonlinear inverse problem

Solution of

$$\min_{x \in \mathbb{R}^n, y \in \mathbb{R}^p} \|A(y)x - b\|_2, \quad \text{where} \quad A(y_{\text{true}})x_{\text{true}} + e = b$$

and

$b \in \mathbb{R}^m$	available observations or measurements
$x_{\text{true}} \in \mathbb{R}^n$	unknown quantity of interest
$y_{\text{true}} \in \mathbb{R}^p$	unknown parameters defining A , $p \ll n$
$A(y) \in \mathbb{R}^{m \times n}$	ill-conditioned matrix models forward process
$e \in \mathbb{R}^m$	additive Gaussian white noise

Example: [image \(semi-\)blind deblurring](#), with Gaussian PSF $P(y)$

$$[P(y)]_{i,j} = c(\sigma_1, \sigma_2, \rho) \exp \left(-\frac{1}{2} \begin{bmatrix} i - \chi_1 \\ j - \chi_2 \end{bmatrix}^T \begin{bmatrix} \sigma_1^2 & \rho^2 \\ \rho^2 & \sigma_2^2 \end{bmatrix}^{-1} \begin{bmatrix} i - \chi_1 \\ j - \chi_2 \end{bmatrix} \right)$$

Note: $\sigma_1^2 \sigma_2^2 - \rho^4 > 0$; $\sum_{i,j=1}^N [P(y)]_{i,j} = 1$.

Here $y = [\sigma_1, \sigma_2, \rho]^T \in \mathbb{R}^3$. For illustrations: $y_{\text{true}} = [2.5, 2.5, 0]^T$.

Dealing with ill-posedness: introducing regularization

- For (large-scale) linear inverse problems
 - early termination of Krylov methods (LSQR, CGLS...), applied to

$$\min_x \|Ax - b\| \quad (\text{from now on, } \|\cdot\| = \|\cdot\|_2)$$

- combining variational (e.g., Tikhonov) regularization methods

$$z_\lambda = \arg \min_{z \in \mathbb{R}^n} \|Az - r_0\|^2 + \lambda^2 \|z\|^2, \quad \text{where} \quad \begin{array}{l} r_0 = b - Ax_0 \\ x_\lambda = x_0 + z_\lambda \end{array}$$

and Krylov methods... equivalently

- first project then regularize
- first regularize then project

Main ingredient (for hybrid solvers): shift-invariance of Krylov subspaces

$$\mathcal{K}_k(A^T A, A^T r_0) = \mathcal{K}_k(A^T A + \lambda^2 I, A^T r_0)$$

See papers by: Bjorck, Buccini, Calvetti, Chung, Donatelli, Espanol, Fenu, G., Hansen, Hanke, Hnetyukova, Hochstenbach, Kilmer, Morigi, Nagy, Novati, O'Leary, Renaut, Reichel, Sgallari

Dealing with ill-posedness: introducing regularization

- For (large-scale) **separable nonlinear inverse problems**

$$(z_\lambda, y^*) = \arg \min_{z \in \mathbb{R}^n, y \in \mathbb{R}^p} \|A(y)z - r_0\|^2 + \lambda^2 \|z\|^2, \quad \text{where} \quad \begin{array}{l} r_0 = b - A(y)x_0 \\ x_\lambda = x_0 + z_\lambda \end{array}$$

Trick: exploit separability!

In particular: apply the **variable projection method** (inner-outer iterations)

- implicitly 'eliminates' z (hybrid solver)
- y is updated using a NLLS solver (e.g., Gauss–Newton)

[Golub and Pereyra, *Inverse Problems*, 2003] [Chung and Nagy, *SISC*, 2010]

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- ***In this talk:***

- introduce inexact Krylov methods (iLSQR, iCGLS) for regularization
- introducing hybrid iLSQR and hybrid iCGLS for regularization
- adopting inexact solvers within the variable projection method (application to blind deblurring)

Transitioning from exact to inexact Golub–Kahan

Inspired by: [Simoncini and Szyld, *SIMAX*, 2003], [Gaaf and Simoncini, *Appl.Num.Math.*, 2017]

exact (GKB)

inexact (iGK)

'iteration-wise'

$$u_1 = r_0/\beta, \quad v_1 = A^T u_1/\alpha_1$$

$$u_{i+1} = (Av_i - \alpha_i u_i)/\beta_{i+1}$$

$$v_{i+1} = (A^T u_{i+1} - \beta_{i+1} v_i)/\alpha_{i+1}$$

$$u_1 = r_0/\beta, \quad v_1 = (A + F_1)^T u_1/[L_{k+1}]_{1,1}$$

$$u_{i+1} = (I - U_i U_i^T)(A + E_i) v_i/[M_k]_{i+1,i+1}$$

$$v_{i+1} = (I - V_i V_i^T)(A + F_{i+1})^T u_{i+1}/[L_{k+1}]_{i+1,i+1}$$

'factorization-wise'

$$AV_k = U_{k+1} \bar{B}_k$$

$$A^T U_{k+1} = V_{k+1} B_{k+1}^T$$

$$\text{where } V_{k+1} = [v_1, \dots, v_{k+1}], \quad U_{k+1} = [u_1, \dots, u_{k+1}]$$

$$[(A + E_1)v_1, \dots, (A + E_k)v_k] = U_{k+1} M_k$$

$$[(A + F_1)^T u_1, \dots, (A + F_{k+1})^T u_{k+1}] = V_{k+1} L_{k+1}^T$$

'compactly factorization-wise'

$$(A + \mathcal{E}_k)V_k = U_{k+1} M_k$$

$$(A + \mathcal{F}_{k+1})^T U_{k+1} = V_{k+1} L_{k+1}^T$$

$$\text{where } \mathcal{E}_k = \sum_{i=1}^k E_i v_i v_i^T$$

$$\mathcal{F}_{k+1} = \sum_{i=1}^{k+1} (u_i u_i^T) F_i$$

links with symmetric Lanczos

$$A^T A V_k = V_{k+1} B_{k+1}^T \bar{B}_k$$

$$(A^T A + \mathcal{F}_{k+1}^T A + A^T \mathcal{E}_k + \mathcal{F}_{k+1}^T \mathcal{E}_k) V_k = V_{k+1} L_{k+1}^T M_k$$

Transitioning from exact to inexact linear system solvers

Inspired by: [Simoncini and Szyld, *SIMAX*, 2003]

$$x_k = x_0 + z_k = x_0 + V_k s_k$$

$$\text{GKB: } AV_k = U_{k+1} \bar{B}_k, \dots$$

LSQR

$$q_k = \arg \min_{q \in \mathcal{R}(U_{k+1} \bar{B}_k) = \mathcal{R}(AV_k)} \|q - r_0\|$$

$$s_k = \arg \min_{s \in \mathbb{R}^k} \|\bar{B}_k s - \beta e_1\|$$

$$(\bar{B}_k^T \bar{B}_k) s_k = \bar{B}_k^T (\beta e_1)$$

$$\text{iGK: } (A + \mathcal{E}_k) V_k = U_{k+1} M_k, \dots$$

inexact LSQR (iLSQR)

$$q_k = \arg \min_{q \in \mathcal{R}(U_{k+1} M_k)} \|q - r_0\|$$

equivalently

$$s_k = \arg \min_{s \in \mathbb{R}^k} \|M_k s - \beta e_1\|$$

does not minimize the true residual!

equivalently

$$(M_k^T M_k) s_k = M_k^T (\beta e_1)$$

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equivalently, **CGLS**

$$V_k^T (A^T A) V_k s_k = V_k^T A^T r_0 = \bar{B}_k^T \beta e_1$$

equivalently

$$q_k \in \mathcal{R}(V_{k+1} \bar{T}_k), A^T r_0 - q_k \perp \mathcal{R}(V_k)$$

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inexact LSQR (iLSQR)

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$$q_k \in \mathcal{R}(V_{k+1} \bar{T}_k), A^T r_0 - q_k \perp \mathcal{R}(V_k)$$

$$\text{iGK: } (A + \mathcal{E}_k) V_k = U_{k+1} M_k, \dots$$

inexact LSQR (iLSQR)

$$q_k = \arg \min_{q \in \mathcal{R}(U_{k+1} M_k)} \|q - r_0\|$$

equivalently

$$s_k = \arg \min_{s \in \mathbb{R}^k} \|M_k s - \beta e_1\|$$

does not minimize the true residual!

equivalently

$$(M_k^T M_k) s_k = M_k^T (\beta e_1)$$

inexact CGLS (iCGLS)

$$q_k \in \mathcal{R}(V_{k+1} \hat{H}_k), (A + \mathcal{F}_{k+1})^T r_0 - q_k \perp \mathcal{R}(V_k)$$

not orthogonal to the true NE residual!

equivalently

$$V_k^T (\hat{A} + \hat{\mathcal{E}}_k) V_k s_k = V_k^T (A + \mathcal{F}_{k+1})^T r_0$$

equivalently

$$\bar{L}_k^T M_k s_k = [\bar{L}_k]_{1,1} \beta e_1$$

Transitioning from inexact linear system solvers to inexact hybrid solvers

Recall, iGK: $(A + \mathcal{E}_k)V_k = U_{k+1}M_k$, $(A + \mathcal{F}_{k+1})^T U_{k+1} = V_{k+1}L_{k+1}^T$

$$x_{\lambda,k} = x_0 + z_{\lambda,k} = x_0 + V_k s_{\lambda,k}$$

λ fixed

inexact LSQR (iLSQR)

$$q_k = \arg \min_{q \in \mathcal{R}(U_{k+1}M_k)} \|q - r_0\|$$

inexact hybrid LSQR (hybrid-iLSQR)

$$q_{\lambda,k} = \arg \min_{q \in \mathcal{R}(W_{\lambda,k})} \left\| q - \begin{bmatrix} r_0 \\ 0 \end{bmatrix} \right\|,$$

$$W_{\lambda,k} = \left[(U_{k+1}M_k)^T, \lambda(V_k)^T \right]^T$$

inexact CGLS (iCGLS)

$$q_k \in \mathcal{R}(V_{k+1}\bar{T}_k), A^T r_0 - q_k \perp \mathcal{R}(V_k)$$

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$$q_{\lambda,k} \in \mathcal{R}(W_{\lambda,k}) = \mathcal{R}(V_{k+1}(\hat{H}_k + \lambda^2 \bar{T})),$$

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equivalently

$$s_{\lambda,k} = \arg \min_{s \in \mathbb{R}^k} \|M_k s - \beta e_1\|^2 + \lambda^2 \|s\|^2$$

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$x_{\lambda,k} = x_0 + z_{\lambda,k} = x_0 + V_k s_{\lambda,k}$

λ fixed: **shift-invariance only under some conditions!**

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When are inexact solvers 'meaningful'?

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Inspired by: [Simoncini and Szyld, *SIMAX*, 2003]

Depends on the relations between exact (i.e., r^e , $r_{\lambda,k}^e$) and inexact (i.e., r , $r_{\lambda,k}$) residuals, keeping in mind that:

- there is ill-posedness: r^e may not be small
- there is regularization: $r_{\lambda,k}^e$ may not be small

$$\text{(i.e., } \|r_{\lambda,k}^e\| = (\|Az_{\text{true}} - r_0^e\|^2 + \lambda^2 \|z_{\text{true}}\|^2)^{1/2} = (\|e\|^2 + \lambda^2 \|z_{\text{true}}\|^2)^{1/2})$$

When are inexact solvers 'meaningful'?

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Focusing on:

- **iLSQR**: $\|r_k^e\| \leq \|r_k\| + \|E_0 x_0\| + \sum_{l=1}^k \|E_l\| \|[s_k]_l\|$
- **hybrid-iLSQR**, fixed λ

$$\|r_{\lambda,k}^e\| \leq \|r_{\lambda,k}\| + \|E_0 x_0\| + \sum_{l=1}^k \|E_l\| \|[s_{\lambda,k}]_l\|$$

'A priori' bounds, ϵ desired accuracy:

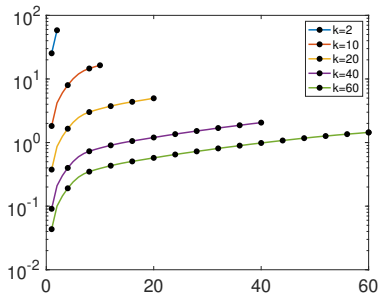
- **iLSQR**: $\|E_j\| \leq \frac{\sigma_k(M_k)}{k} \frac{1}{\|r_{j-1}\|} \epsilon$, $j = 1, \dots, k$
- **hybrid-iLSQR**, fixed λ

$$\|E_j\| \leq \frac{(\sigma_k(M_k^T M_k + \lambda^2 I))^{1/2}}{k} \frac{1}{\|r_{\lambda,j-1}\|} \epsilon, \quad j = 1, \dots, k$$

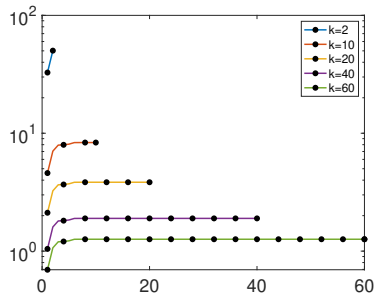
An illustration

satellite blind deblurring example, with $\lambda = 0.5$

$$\frac{\sigma_k(M_k)}{k} \frac{1}{\|r_{j-1}\|} \text{ vs. } j$$



$$\frac{(\sigma_k(M_k^T M_k + \lambda^2 I))^{1/2}}{k} \frac{1}{\|r_{\lambda,j-1}\|} \text{ vs. } j$$



Recap on separable NLLS and VarPro

[Golub and Pereyra, *Inverse Problems*, 2003] [Chung and Nagy, *SISC*, 2010]

■ Problem to be solved

$$z_\lambda = \arg \min_{z \in \mathbb{R}^n, y \in \mathbb{R}^p} g(z, y), \text{ where}$$

$$\begin{aligned} g(z, y) &= \|F(z, y)\|^2 \\ F(z, y) &= \tilde{A}_\lambda(y)z - \tilde{r}_0 \\ \tilde{A}_\lambda(y) &= [A^T(y), \lambda I]^T, \tilde{r}_0 = [r_0^T, 0^T]^T \\ x_\lambda &= x_0 + z_\lambda \end{aligned}$$

■ Consider the reduced cost functional

$$h(y) := g(z_\lambda(y), y), \quad \text{where} \quad \begin{aligned} z_\lambda(y) &= \arg \min_{z \in \mathbb{R}^n} g(z, y) \\ &= (A^T(y)A(y) + \lambda^2 I)^{-1} A^T(y)r_0 \end{aligned}$$

Take $x_\lambda(y) = x_0 + z_\lambda(y)$

■ Apply Gauss-Newton to minimize the reduced cost functional

$$y_l = y_{l-1} + \gamma_l d_{l-1} \quad (\text{setting the steplength } \gamma_l)$$

Note that

$$d_{l-1} = \arg \min_d \|\hat{J}_h d - r_{l-1}\|, \quad J_h = \begin{bmatrix} d(A(y)z_\lambda)/dy \\ 0 \end{bmatrix} = \begin{bmatrix} \hat{J}_h \\ 0 \end{bmatrix}, \quad J_h^T F(z_\lambda, y) = \nabla_y g(z_\lambda, y)$$

(computationally convenient analytical expression of $d(A(y)z_\lambda)/dy$ for blind deblurring)

Towards an iGK-based algorithm for separable nonlinear least squares problems

[Chung and Nagy, *SISC*, 2010]

Algorithm Variable projection with Gauss-Newton and *hybrid LSQR* solver

- 1: Choose initial guesses x_0 and y_0
 - 2: **for** $l = 1, 2, \dots$ until a stopping criterion is satisfied **do**
 - 3: **for** $k = 1, 2, \dots$ until a stopping criterion is satisfied **do**
 - 4: Expand $\mathcal{K}_k(A(y_{l-1})^T A(y_{l-1}), A(y_{l-1})^T r_0)$ using **GKB**
 - 5: Compute $x_{\lambda,k}$ solving the projected problem with adaptive choice of λ
 - 6: **end for**
 - 7: Compute the residual $r_l = b - A(y_{l-1})x_{\lambda,k}$
 - 8: Compute $d_l = \arg \min_d \|\widehat{J}_h d - r_l\|$
 - 9: Update $y_l = y_{l-1} + \gamma_l d_l$ (setting the steplength γ_l)
 - 10: Update x_0
 - 11: **end for**
-

Towards an iGK-based algorithm for separable nonlinear least squares problems

Algorithm Variable projection with Gauss-Newton and *hybrid LSQR* solver

- 1: Choose initial guesses x_0 and y_0
 - 2: ~~for $l = 1, 2, \dots$ until a stopping criterion is satisfied do~~
 - 3: **for** $k = 1, 2, \dots$ until a stopping criterion is satisfied **do**
 - 4: Expand $\mathcal{K}_k(A(y_{l-1})^T A(y_{l-1}), A(y_{l-1})^T r_0)$ using GKB
 - 5: Compute $x_{\lambda,k}$ solving the projected problem with adaptive choice of λ
 - 6: **end for**
 - 7: Compute the residual $r_l = b - A(y_{l-1})x_{\lambda,k}$
 - 8: Compute $d_l = \arg \min_d \|\widehat{J}_h d - r_l\|$
 - 9: Update $y_l = y_{l-1} + \gamma_l d_l$ (setting the steplength γ_l)
 - 10: Update x_0
 - 11: ~~end for~~
-

Towards an iGK-based algorithm for separable nonlinear least squares problems

Algorithm Variable projection with Gauss-Newton and *hybrid-iLSQR* solver

Choose initial guesses x_0 and y_0

for $k = 1, 2, \dots$ until inexactness exceeds the bound ε **do**

 Expand the approximation subspace $\mathcal{R}(V_k)$ using $A(y_{k-1})$ and **iGK**

 Compute $x_{\lambda,k}$ solving the projected problem with adaptive choice of λ

 Compute the residual $r_k = b - A(y_{k-1})x_{\lambda,k}$

 Compute $d_k = \arg \min_d \|\hat{J}_h d - r_k\|$

 Update $y_k = y_{k-1} + \gamma_k d_k$ (setting the steplength γ_k)

end for

Towards an iGK-based algorithm for separable nonlinear least squares problems

Algorithm Variable projection with Gauss-Newton and *hybrid-iLSQR* solver

- 1: Choose initial guesses x_0 and y_0 ; set an accuracy ε
 - 2: for $l = 1, 2, \dots$ until a stopping criterion is satisfied do
 - 3: **for** $k = 1, 2, \dots$ until inexactness exceeds the bound ε **do**
 - 4: Expand the approximation subspace $\mathcal{R}(V_k)$ using $A(y_{k-1})$ and **iGK**
 - 5: Compute $x_{\lambda,k}$ solving the projected problem with adaptive choice of λ
 - 6: Compute the residual $r_k = b - A(y_{k-1})x_{\lambda,k}$
 - 7: Compute $d_k = \arg \min_d \|\widehat{J}_h d - r_k\|$
 - 8: Update $y_k = y_{k-1} + \gamma_k d_k$ (setting the steplength γ_k)
 - 9: **end for**
 - 10: Update x_0 ; take $y_0 = y_k$
 - 11: **end for**
-

A few details

■ Defining inexactness, with some pragmatism:

consider as exact matrix the latest computed approximation of $A(y)$, i.e.,

after $j - 1$ iterations, $A(y_{j-1}) = A(y_{j-1}) + E_j^j$, where $E_j^j := A(y_{j-1}) - A(y_{j-1})$,

iGK being expressed as

$$\begin{aligned} (A(y_{j-1}) + E_j^j) V_j &= U_{j+1} M_j, & E_j^j &= \sum_{i=1}^j E_i^j v_i v_i^T \\ (A(y_{j-1}) + F_{j+1}^j)^T U_{j+1} &= V_{j+1} L_{j+1}^T, & F_{j+1}^j &= \sum_{i=1}^{j+1} u_i u_i^T E_{i-1}^j \end{aligned}$$

■ Setting the Gauss-Newton stepsize: set

$$y_j = y_{j-1} + \gamma_j d_{j-1}, \quad \text{where } \gamma_j = \arg \min_{\gamma \geq 0} g(z_\lambda(y_{j-1}), y_{j-1} + \gamma d_{j-1})$$

We get

$$\|\tilde{A}_\lambda(y_j) z_{\lambda,j+1} - \tilde{r}_0\| \leq \|\tilde{A}_\lambda(y_{j-1}) z_{\lambda,j} - \tilde{r}_0\| + 2\tilde{\varepsilon},$$

instead of

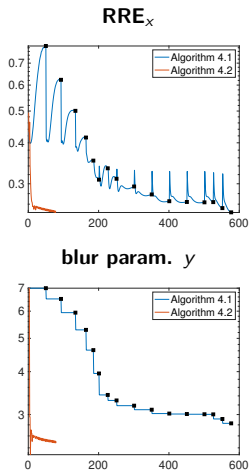
$$\|\tilde{A}_\lambda(y_j) z_{\lambda,j+1} - \tilde{r}_0\| \leq \|\tilde{A}_\lambda(y_{j-1}) z_{\lambda,j} - \tilde{r}_0\|$$

An illustration

satellite blind deblurring example, with $y_{\text{true}} = [2.5, 2.5, 0]^T$, $\lambda = 0.5$

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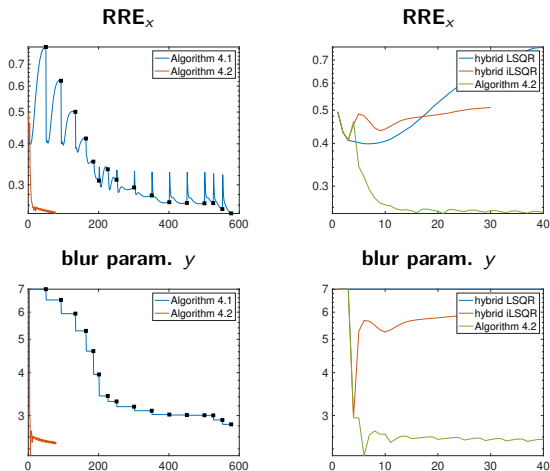
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Algorithm 4.1: [Chung and Nagy, *SISC*, 2010]; Algorithm 4.2: new solver

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An illustration

Hybrid-iLSQR

(it. 30, RRE_x 0.5819)



Algorithm 4.1

(it. 577, RRE_x 0.2454)



Algorithm 4.2

(it. 79, RRE_x 0.2474)



Algorithm 4.1: [Chung and Nagy, *SISC*, 2010]; Algorithm 4.2: new solver

Another example

cameraman blind deblurring example, with $y_{\text{true}} = [3, 4, 0.5]^T$, $y_0 = [5, 6, 1]^T$

exact



Algorithm 4.1

(it. 927, RRE_v 0.1286)



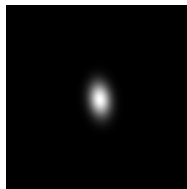
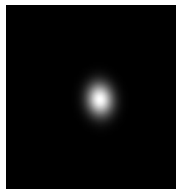
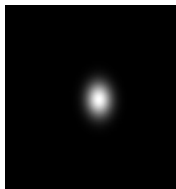
(it. 927, RRE_v 0.0679)

Algorithm 4.2

(it. 82, RRE_v 0.1219)



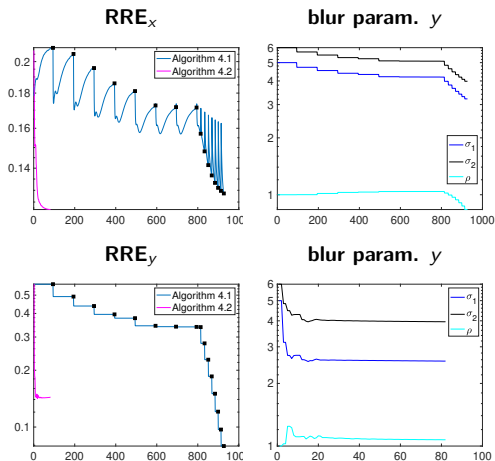
(it. 82, RRE_v 0.1438)



Algorithm 4.1: [Chung and Nagy, *SISC*, 2010]; Algorithm 4.2: new solver

Another example

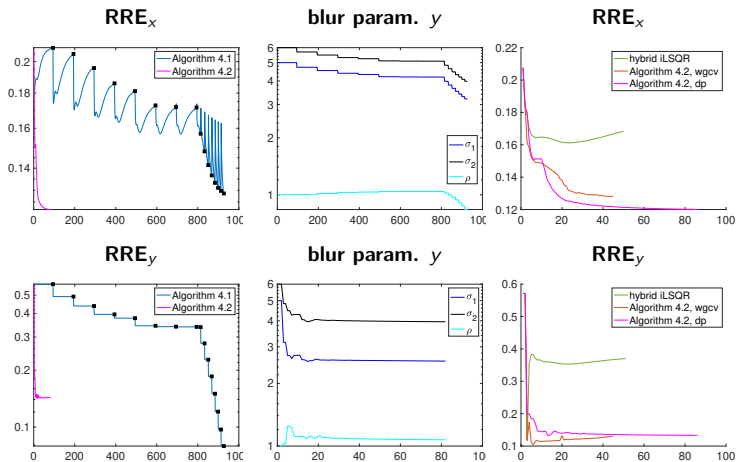
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Thanks for your attention!

Silvia Gazzola and Malena Sabaté Landman
*Regularization by inexact Krylov methods
with applications to blind deblurring*
SIAM J. Matrix Anal. Appl. 42, 2021