Regularization by inexact Krylov methods

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Setting the stage: linear inverse problem

Solution of

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

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
$\mathrm{e}\in\mathbb{R}^m$	additive Gaussian white noise

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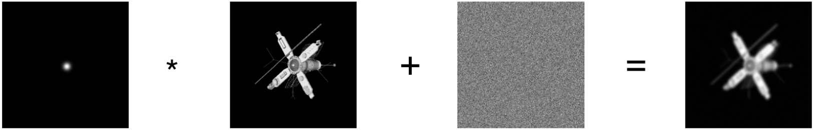
$e \in \mathbb{R}^m$	additive Gaussian white noise

Example: image deblurring



PSF * exact + noise = data

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

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

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

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

    and Krylov methods... equivalently
    - first project then regularize
    - first regularize then project

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

$$\mathcal{K}_k(A^TA, A^Tr_0) = \mathcal{K}_k(A^TA + \lambda^2 I, A^Tr_0)$$

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

Dealing with ill-posedness: introducing regularization

- For (large-scale) separable nonlinear inverse problems

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

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]

Dealing with ill-posedness: introducing regularization

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

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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'

exact (GKB):

$$u_1 = r_0/\beta,\ v_1 = A^T u_1/\alpha_1$$
$$u_{i+1} = (Av_i - \alpha_i u_i)/\beta_{i+1}$$
$$v_{i+1} = (A^T u_{i+1} - \beta_{i+1} v_i)/\alpha_{i+1}$$

inexact (iGK):

$$u_1 = r_0/\beta,\ v_1 = (A + F_1)^T u_1/[L_{k+1}]_{1,1}$$
$$u_{i+1} = (I - U_i U_i^T)(A + E_i)v_i/[M_k]_{i+1,i+1}$$
$$v_{i+1} = (I - V_i V_i^T)(A + F_{i+1})^T u_{i+1}/[L_{k+1}]_{i+1,i+1}$$

'factorization-wise'

exact (GKB):

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

inexact (iGK):

$$[(A+E_1)v_1, \dots, (A+E_k)v_k] = U_{k+1}M_k$$
$$\left[(A+F_1)^T u_1, \dots, (A+F_{k+1})^T u_{k+1}\right] = V_{k+1}L_{k+1}^T$$

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

'compactly factorization-wise'

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

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

exact (GKB):

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

inexact (iGK):

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

Transitioning from exact to inexact linear system solvers

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

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

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

LSQR

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

equivalently

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

equivalently

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

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

inexact LSQR (iLSQR)

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

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

does not minimize the true residual!

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

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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

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

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

LSQR

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equivalently

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

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equivalently

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

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)

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

not orthogonal to the true NE residual!

equivalently

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

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)

$$q_{\lambda,k} = \arg\min_{q\in\mathcal{R}(W_{\lambda,k})} \left\| q - \begin{bmatrix} r_0 \\ 0 \end{bmatrix} \right\|, \quad W_{\lambda,k} = \left[(U_{k+1}M_k)^T, \lambda(V_k)^T\right]^T$$

inexact CGLS (iCGLS)

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

inexact hybrid CGLS (hybrid-iCGLS)

$$q_{\lambda,k} \in \mathcal{R}(W_{\lambda,k}) = \mathcal{R}(V_{k+1}(\widehat{H}_k + \lambda^2\bar{I})),$$
$$(A+\mathcal{F}_{k+1})^T r_0 - q_{\lambda,k} \perp \mathcal{R}(V_k)$$

Transitioning from inexact linear system solvers to inexact hybrid solvers

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

$$\begin{aligned} s_{\lambda,k} &= \arg\min_{s\in\mathbb{R}^k} \|M_k s - \beta e_1\|^2 + \lambda^2\|s\|^2 \\ &= (M_k^T M_k + \lambda^2 I)^{-1} M_k^T(\beta e_1) \end{aligned}$$

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equivalently

$$(\bar{L}_k^T M_k + \lambda^2 I)s_{\lambda,k} = [\bar{L}_k]_{1,1}\beta e_1$$

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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: shift-invariance only under some conditions!

inexact LSQR (iLSQR)

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

inexact hybrid LSQR (hybrid-iLSQR)

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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, $r^e_{\lambda,k}$) 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: $r^e_{\lambda,k}$ may not be small
  (i.e., $\left\| r^e_{\lambda,k} \right\| = \left(\|Az_{\text{true}} - r^e_0\|^2 + \lambda^2 \|z_{\text{true}}\|^2 \right)^{1/2} = \left(\|e\|^2 + \lambda^2 \|z_{\text{true}}\|^2 \right)^{1/2}$)

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Focusing on:

- **iLSQR**: $\|r^e_k\| \leq \|r_k\| + \|E_0x_0\| + \sum_{l=1}^k \|E_l\| \, |[s_k]_l|$
- **hybrid-iLSQR**, fixed λ

$$\left\|r^e_{\lambda,k}\right\| \leq \|r_{\lambda,k}\| + \|E_0x_0\| + \sum_{l=1}^{k} \|E_l\| |[s_{\lambda,k}]_l|$$

'A priori' bounds, ϵ desired accuracy:

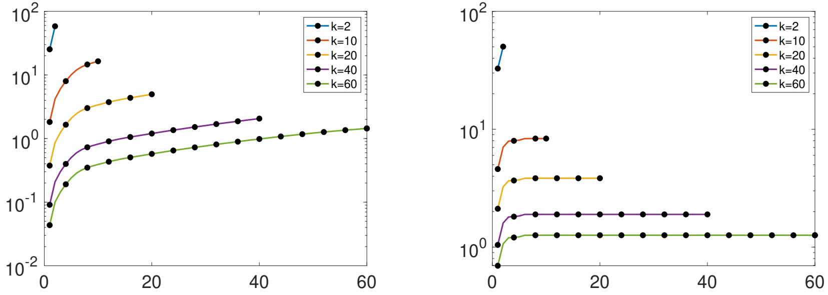
- **iLSQR**: $\|E_j\| \leq \dfrac{\sigma_k(M_k)}{k} \frac{1}{\|r_{j-1}\|}\epsilon$, $j = 1, \ldots, k$
- **hybrid-iLSQR**, fixed λ

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

An illustration

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

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



Recap on separable NLLS and VarPro

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

- Problem to be solved

$$z_\lambda = \arg\min_{z\in\mathbb{R}^n, y\in\mathbb{R}^p} g(z,y)\,,\ \text{where}\ \begin{array}{lcl} g(z,y) &=& \|F(z,y)\|^2 \\ F(z,y) &=& \widetilde{A}_\lambda(y)z - \widetilde{r}_0 \\ \widetilde{A}_\lambda(y) &=& [A^T(y), \lambda I]^T,\ \widetilde{r}_0 = [r_0^T, 0^T]^T \\ x_\lambda &=& x_0 + z_\lambda \end{array}$$

- Consider the reduced cost functional

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

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

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

(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

```
Choose initial guesses x_0 and y_0
for l = 1, 2, ... until a stopping criterion is satisfied do
    for k = 1, 2, ... until a stopping criterion is satisfied do
        Expand K_k(A(y_{l-1})^T A(y_{l-1}), A(y_{l-1})^T r_0) using GKB
        Compute x_{λ,k} solving the projected problem with adaptive choice of λ
    end for
    Compute the residual r_l = b - A(y_{l-1}) x_{λ,k}
    Compute d_l = arg min_d ||Ĵ_h d - r_l||
    Update y_l = y_{l-1} + γ_l d_l (setting the steplength γ_l)
    Update x_0
end for
```

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

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

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

iGK being expressed as

$$
\begin{aligned}
(A(y_{j-1}) + \mathcal{E}_j^j)V_j &= U_{j+1}M_j, & \mathcal{E}_j^j &= \textstyle\sum_{i=1}^j E_i^j v_i v_i^T \\
(A(y_{j-1}) + \mathcal{F}_{j+1}^j)^T U_{j+1} &= V_{j+1}L_{j+1}^T, & \mathcal{F}_{j+1}^j &= \textstyle\sum_{i=1}^{j+1} u_i u_i^T E_{i-1}^j
\end{aligned}
$$

- Setting the Gauss-Newton stepsize:

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

We get

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

instead of

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

An illustration

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

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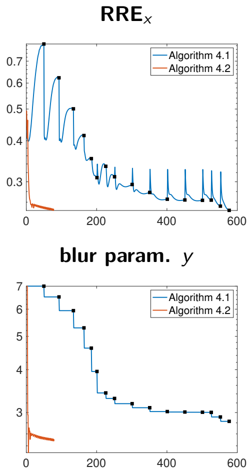

Algorithm 4.1: [Chung and Nagy, *SISC*, 2010]; Algorithm 4.2: new solver

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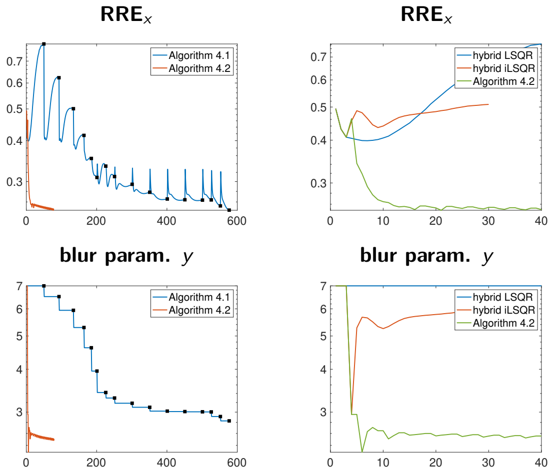


Algorithm 4.1: [Chung and Nagy, *SISC*, 2010]; Algorithm 4.2: new solver

An illustration

Hybrid-iLSQR
(it. 30, RRE_x 0.5819)

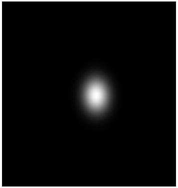
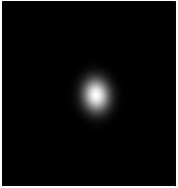
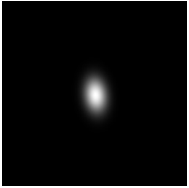
Algorithm 4.1
(it. 577, RRE_x 0.2454)

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**	**Algorithm 4.2**
	(it. 927, RRE_x 0.1286)	(it. 82, RRE_x 0.1219)
		
	(it. 927, RRE_y 0.0679)	(it. 82, RRE_y 0.1438)
		

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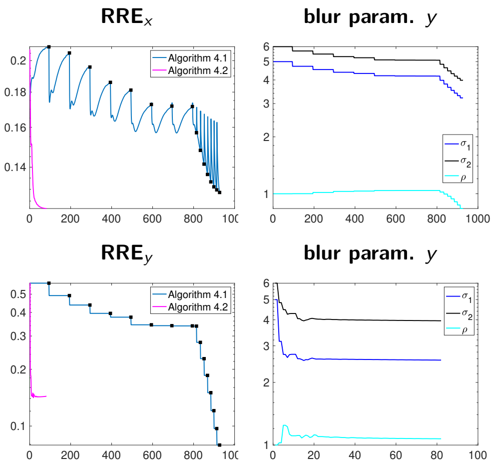

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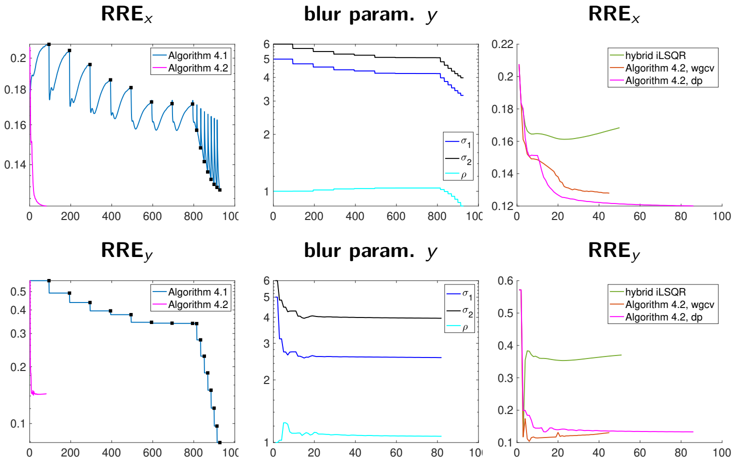

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Thanks for your attention!

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