Test problems

Iterative Solvers

Conclusions

Introducing IR Tools

Silvia Gazzola Joint work with P. C. Hansen and J. Nagy

Department of Mathematical Sciences



LMS – EPSRC Durham Symposium, Model Order Reduction August 15, 2017

Test problems

Iterative Solvers

Outline

1 Introduction

- Discrete inverse problems
- Putting IR Tools into place

2 Test problems

- Image deblurring
- Computed tomography
- Inverse Interpolation

3 Iterative Solvers

- Enhancing classical iterative methods
- Regularization, projection, hybrid methods

4 Conclusions

Test problems

Iterative Solvers

Conclusions

Some backrgound

Iterative Solvers

Some backrgound

- discretization of Fredholm integral equation of the first kind
- $A \in \mathbb{R}^{M \times N}$, $b \in \mathbb{R}^{M}$
- e unknown noise

Iterative Solvers

Some backrgound

Numerical solution of $Ax^* + e = b$

discretization of Fredholm integral equation of the first kind

•
$$A \in \mathbb{R}^{M imes N}$$
, $b \in \mathbb{R}^N$

- e unknown noise
- ill-posed

Some backrgound

Numerical solution of $Ax^* + e = b$

discretization of Fredholm integral equation of the first kind

$$A \in \mathbb{R}^{M imes N}$$
, $b \in \mathbb{R}^{N}$

- e unknown noise
- ill-posed (looking at the SVD of $A = U\Sigma V^T$)

Introd	uction
000	

Conclusions

Some backrgound

- discretization of Fredholm integral equation of the first kind
- $A \in \mathbb{R}^{M \times N}$, $b \in \mathbb{R}^{M}$
- e unknown noise
- ill-posed (looking at the SVD of $A = U\Sigma V^T$)



Introd	uction
000	

Conclusions

Some backrgound

- discretization of Fredholm integral equation of the first kind
- $A \in \mathbb{R}^{M \times N}$, $b \in \mathbb{R}^{M}$
- e unknown noise
- ill-posed (looking at the SVD of $A = U\Sigma V^T$)



Introd	uction
000	

Conclusions

Some backrgound

- discretization of Fredholm integral equation of the first kind
- $A \in \mathbb{R}^{M \times N}$, $b \in \mathbb{R}^{M}$
- e unknown noise
- ill-posed (looking at the SVD of $A = U\Sigma V^T$)



Test problems

Iterative Solvers

Conclusions

Applying some regularization

Introd	uction
000	

Conclusions

Applying some regularization

- "small-scale" problems (direct)
 - TSVD
 - Tikhonov-regularization

$$\min_{x} \left\{ \|Ax - b\|_{2}^{2} + \lambda^{2} \Omega(x) \right\}, \quad \Omega(x) = \|x\|_{2}^{2}, \ \|Lx\|_{2}^{2}$$

Introd	uction
000	

Conclusions

Applying some regularization

- "small-scale" problems (direct)
 - TSVD
 - Tikhonov-regularization

$$\min_{x} \left\{ \|Ax - b\|_{2}^{2} + \lambda^{2} \Omega(x) \right\}, \quad \Omega(x) = \|x\|_{2}^{2}, \ \|Lx\|_{2}^{2}$$

"large-scale" problems (iterative)

Introd	uction
000	

Conclusions

Applying some regularization

- "small-scale" problems (direct)
 - TSVD
 - Tikhonov-regularization

$$\min_{x} \left\{ \|Ax - b\|_{2}^{2} + \lambda^{2} \Omega(x) \right\}, \quad \Omega(x) = \|x\|_{2}^{2}, \ \|Lx\|_{2}^{2}$$

- "large-scale" problems (iterative)
 - iterative regularization: semi-convergence and early stopping



Introd	uction
000	

Conclusions

Applying some regularization

- "small-scale" problems (direct)
 - TSVD
 - Tikhonov-regularization

$$\min_{x} \left\{ \|Ax - b\|_{2}^{2} + \lambda^{2} \Omega(x) \right\}, \quad \Omega(x) = \|x\|_{2}^{2}, \ \|Lx\|_{2}^{2}$$

- "large-scale" problems (iterative)
 - iterative regularization: semi-convergence and early stopping



S. Gazzola (UoB)

Test problem

Iterative Solvers

Conclusions

Here IR Tools comes...

Test problem

Iterative Solvers

Conclusions

Here IR Tools comes...

"state-of-the-art":

Iterative Solvers

Here IR Tools comes...

"state-of-the-art":

Regularization Tools

P. C. Hansen. Regularization Tools: A Matlab Package for Analysis and Solution of Discrete III-Posed Problems. Numer. Algo., 1994 till 2007.

Restore Tools

J. G. Nagy, K. Palmer, and L. Perrone. Iterative methods for image deblurring: A Matlab object oriented approach. Numer. Algo., 2004 till 2012.

AIR Tools (II)

P. C. Hansen and M. S. Hansen. AIR Tools – A MATLAB package of algebraic iterative reconstruction methods. JCAM, 2012.

P. C. Hansen and J. S. Jorgensen. AIR Tools II: Algebraic iterative reconstruction meth- ods, improved implementation. Numer. Algo. (submitted), 2017.

Iterative Solvers

Here IR Tools comes...

"state-of-the-art":

Regularization Tools

P. C. Hansen. Regularization Tools: A Matlab Package for Analysis and Solution of Discrete III-Posed Problems. Numer. Algo., 1994 till 2007.

small problems

Restore Tools

J. G. Nagy, K. Palmer, and L. Perrone. Iterative methods for image deblurring: A Matlab object oriented approach. Numer. Algo., 2004 till 2012.

image deblurring problems only.

AIR Tools (II)

P. C. Hansen and M. S. Hansen. AIR Tools – A MATLAB package of algebraic iterative reconstruction methods. JCAM, **2012**.

P. C. Hansen and J. S. Jorgensen. AIR Tools II: Algebraic iterative reconstruction meth- ods, improved implementation. Numer. Algo. (submitted), 2017.

tomography problems only

Iterative Solvers

Here IR Tools comes...

"state-of-the-art":

Regularization Tools

P. C. Hansen. Regularization Tools: A Matlab Package for Analysis and Solution of Discrete III-Posed Problems. Numer. Algo., 1994 till 2007.

small problems

Restore Tools

J. G. Nagy, K. Palmer, and L. Perrone. Iterative methods for image deblurring: A Matlab object oriented approach. Numer. Algo., 2004 till 2012.

image deblurring problems only.

AIR Tools (II)

P. C. Hansen and M. S. Hansen. AIR Tools – A MATLAB package of algebraic iterative reconstruction methods. JCAM, **2012**.

P. C. Hansen and J. S. Jorgensen. AIR Tools II: Algebraic iterative reconstruction meth- ods, improved implementation. Numer. Algo. (submitted), 2017.

tomography problems only

Features and goals of IR Tools:

Iterative Solvers

Here IR Tools comes...

"state-of-the-art":

Regularization Tools

P. C. Hansen. Regularization Tools: A Matlab Package for Analysis and Solution of Discrete III-Posed Problems. Numer. Algo., 1994 till 2007.

small problems

Restore Tools

J. G. Nagy, K. Palmer, and L. Perrone. Iterative methods for image deblurring: A Matlab object oriented approach. Numer. Algo., 2004 till 2012.

image deblurring problems only.

AIR Tools (II)

P. C. Hansen and M. S. Hansen. AIR Tools – A MATLAB package of algebraic iterative reconstruction methods. JCAM, 2012.

P. C. Hansen and J. S. Jorgensen. AIR Tools II: Algebraic iterative reconstruction meth- ods, improved implementation. Numer. Algo. (submitted), 2017.

tomography problems only

Features and goals of IR Tools:

model implementation of a variety of "new" iterative regularization methods;

Iterative Solvers

Here IR Tools comes...

"state-of-the-art":

Regularization Tools

P. C. Hansen. Regularization Tools: A Matlab Package for Analysis and Solution of Discrete III-Posed Problems. Numer. Algo., 1994 till 2007.

small problems

Restore Tools

J. G. Nagy, K. Palmer, and L. Perrone. Iterative methods for image deblurring: A Matlab object oriented approach. Numer. Algo., 2004 till 2012.

image deblurring problems only.

AIR Tools (II)

P. C. Hansen and M. S. Hansen. AIR Tools – A MATLAB package of algebraic iterative reconstruction methods. JCAM, 2012.
P. C. Hansen and J. S. Jorgensen. AIR Tools II: Algebraic iterative reconstruction meth- ods, improved implementation.

P. C. Hansen and J. S. Jorgensen. AIR Tools II: Algebraic iterative reconstruction meth- ods, improved implementation Numer. Algo. (submitted), 2017.

tomography problems only

Features and goals of IR Tools:

- model implementation of a variety of "new" iterative regularization methods;
- new realistic 2D test problems;

Iterative Solvers

Here IR Tools comes...

"state-of-the-art":

Regularization Tools

P. C. Hansen. Regularization Tools: A Matlab Package for Analysis and Solution of Discrete III-Posed Problems. Numer. Algo., 1994 till 2007.

small problems

Restore Tools

J. G. Nagy, K. Palmer, and L. Perrone. Iterative methods for image deblurring: A Matlab object oriented approach. Numer. Algo., 2004 till 2012.

image deblurring problems only.

AIR Tools (II)

 P. C. Hansen and M. S. Hansen. AIR Tools – A MATLAB package of algebraic iterative reconstruction methods. JCAM, 2012.
 P. C. Hansen and J. S. Jorgensen. AIR Tools II: Algebraic iterative reconstruction meth- ods, improved implementation.

Numer. Algo. (submitted), 2017.

tomography problems only

Features and goals of IR Tools:

- model implementation of a variety of "new" iterative regularization methods;
- new realistic 2D test problems;
- easy to use: almost identical calls to iterative solvers and test-problem generators; naming convention for all functions; default options;

Iterative Solvers

Here IR Tools comes...

"state-of-the-art":

Regularization Tools

P. C. Hansen. Regularization Tools: A Matlab Package for Analysis and Solution of Discrete III-Posed Problems. Numer. Algo., 1994 till 2007.

small problems

Restore Tools

J. G. Nagy, K. Palmer, and L. Perrone. Iterative methods for image deblurring: A Matlab object oriented approach. Numer. Algo., 2004 till 2012.

image deblurring problems only.

AIR Tools (II)

 P. C. Hansen and M. S. Hansen. AIR Tools – A MATLAB package of algebraic iterative reconstruction methods. JCAM, 2012.
 P. C. Hansen and J. S. Jorgensen. AIR Tools II: Algebraic iterative reconstruction meth- ods, improved implementation. Numer. Algo. (submitted). 2017.

tomography problems only

Features and goals of IR Tools:

- model implementation of a variety of "new" iterative regularization methods;
- new realistic 2D test problems;
- easy to use: almost identical calls to iterative solvers and test-problem generators; naming convention for all functions; default options;
- flexible (control over the parameters) and expandable.

S. Gazzola (UoB)

Iterative Solvers

Conclusions

Test problems: the PRxxx functions

Generating a test problem:

1 Define A, b^* , x^* .

2 Add noise to
$$b^* = Ax^*$$
: $b = b^* + e$.

3 Visualise the data.

S. Gazzola (UoB)

Test problems: the PRxxx functions

Generating a test problem:

- **1** Define A, b^* , x^* .
 - PRblur

image deblurring: spatially (in)variant blur

- PRtomo, PRspherical, PRseismic computed tomography: X-ray, spherical, seismic travel-time
- PRinvinterp2 inverse interpolation
- PRnmr

nuclear magnetic resonance (NMR)

2 Add noise to
$$b^* = Ax^*$$
: $b = b^* + e$.

3 Visualise the data.

Conclusions

Test problems: the PRxxx functions

Generating a test problem:

- **1** Define *A*, b^* , x^* .
 - PRblur

image deblurring: spatially (in)variant blur

- PRtomo, PRspherical, PRseismic computed tomography: X-ray, spherical, seismic travel-time
- PRinvinterp2 inverse interpolation
- PRnmr

nuclear magnetic resonance (NMR)

- 2 Add noise to $b^* = Ax^*$: $b = b^* + e$. PRnoise (Gauss, Poisson, Multiplicative)
- 3 Visualise the data.

Test problems: the PRxxx functions

Generating a test problem:

- **1** Define *A*, b^* , x^* .
 - PRblur

image deblurring: spatially (in)variant blur

- PRtomo, PRspherical, PRseismic computed tomography: X-ray, spherical, seismic travel-time
- PRinvinterp2 inverse interpolation
- PRnmr

nuclear magnetic resonance (NMR)

- 2 Add noise to $b^* = Ax^*$: $b = b^* + e$. PRnoise (Gauss, Poisson, Multiplicative)
- **3** Visualise the data.
 - PRshowb, PRshowx

S. Gazzola (UoB)

Test problems

Iterative Solvers

Conclusions

Something more about PRblur

Test problems

Iterative Solvers

Conclusions

Something more about PRblur



available

Test problems

Iterative Solvers

Conclusions

Something more about PRblur



PSF



exact

noise



=

available

+

Test problems

Iterative Solvers

Conclusions

Something more about PRblur



PSF



exact

noise



=

available

Basic call:

[A, b, x, ProbInfo] = PRblur;

+

Test problems

Iterative Solvers

Conclusions

Something more about PRblur



PSF



exact





=

available

Basic call:

[A, b, x, ProbInfo] = PRblur;

+

ProbInfo is a struct:

problemType:	$^{\prime} \texttt{deblurring}^{\prime}$
xType :	' image2D'
xSize:	[256 256]
bType :	' image2D'
bSize:	[256 256]
psf:	[256x256double]

Test problems

Iterative Solvers

Conclusions

Something more about PRblur



PSF



exact





=

available

Basic call:

[A, b, x, ProbInfo] = PRblur;

+

ProbInfo is a struct:

problemType:	$^{\prime} \texttt{deblurring}^{\prime}$
xType :	'image2D'
xSize:	[256 256]
bType :	'image2D'
bSize:	[256 256]
psf:	[256x256double]

More advanced call:

[A, b, x, ProbInfo] = PRblur(n, options);

S. Gazzola (UoB)

Test problems

Iterative Solvers

Conclusions

Exploring the PRblur options

Test problems

Iterative Solvers

Conclusions

Exploring the PRblur options

default options (spatially invariant, medium level, reflective b.c.)







Test problems

Iterative Solvers

Conclusions

Exploring the PRblur options

default options (spatially invariant, medium level, reflective b.c.)





.

PSF

shaking blur (spatially variant, mild level, zero b.c.)






Test problems

Iterative Solvers

Conclusions

Exploring the PRblur options

default options (spatially invariant, medium level, reflective b.c.)







shaking blur (spatially variant, mild level, zero b.c.)







 rotation blur (spatially variant, severe level, periodic b.c.) [Hansen, Nagy, and Tigkos. Rotational image deblurring with sparse matrices, BIT, 2014]
 **





S. Gazzola (UoB)

IR Tools intro

August 15, 2017 8 / 18

Something more about PRtomo, PRspherical, PRseismic



X-ray computed tomography (image courtesy: Hansen, Jorgensen, AIR Tools II)



fan. curved



■ X-ray computed tomography (image courtesy: Hansen, Jorgensen, AIR Tools II)



Spherical means tomography (image courtesy: Hansen, Jorgensen, AIR Tools II)





X-ray computed tomography (image courtesy: Hansen, Jorgensen, AIR Tools II)



Spherical means tomography (image courtesy: Hansen, Jorgensen, AIR Tools II)



Seismic travel-time tomography (image courtesy: Hansen, Jorgensen, AIR Tools II)







Iterative Solvers

Conclusions

Exploring the tomographic problems' options

Introduction	Test problems	Iterative Solvers	Conclusion
000	○○○●○	00000	

Exploring the tomographic problems' options

For all the problems: opt.phantomImage

Exploring the tomographic problems' options

For all the problems: opt.phantomImage

[A, b, x, ProbInfo] = PRtomo(n,

Shepp-Logan



opt); choosing CTtype, angles, p... parallel (over)



parallel (under)



 Introduction
 Test problems
 Iterative Solvers
 Conclusions

 000
 00000
 00000
 Conclusions

 Exploring the tomographic problems' options
 00000
 Conclusions





[A, b, x, ProbInfo] = PRseismic(n, opt); choosing wavemodel, p...
smooth





	tr							
	~	~	~	-	~	-	~	
0								

Test problems

Iterative Solvers

Conclusions

Introduction	Test problems	Iterative Solvers	Con
000	○○○○●	00000	
C	1		



Intro	du	cti	on

Test problems

Iterative Solvers

Conclusions



Test problems

Iterative Solvers

Conclusions



Test problems

Iterative Solvers

Conclusions



Test problems

Iterative Solvers

Conclusions



	a la sust. DD i sustante		
Introduction	Test problems	Iterative Solvers	Conclusions
000	○○○○●	00000	

Something more about PRinvinterp



options.InterpMethod: 'linear', 'nearest', 'cubic', 'spline'.

Test problem

Iterative Solvers

Conclusions

Iterative Solvers: the IRxxx functions

$$\begin{split} \min_{x \in \mathbb{R}^N} \|Ax - b\|_2^2 & (\text{LS}) \\ \min_{x \in \mathbb{R}^N} \|Ax - b\|_2^2 + \lambda^2 \Omega(x) & (\text{cLS}) \end{split}$$

Test problem

Iterative Solvers

Conclusions

Iterative Solvers: the IRxxx functions

$$\begin{split} \min_{x \in \mathbb{R}^N} & \|Ax - b\|_2^2 \qquad (\text{LS}) \\ \min_{x \in \mathbb{R}^N} & \|Ax - b\|_2^2 + \lambda^2 \Omega(x) \qquad (\text{cLS}) \end{split}$$

solver	problem	notes
IRart	(LS)	
IRsirt	(LS)	
IRmrnsd	(LS)	$x \ge 0$
IRfista	(cLS)	$x \in \mathcal{C}$, $\Omega(x) = \ x\ _1$
Krylov methods		
TRagla	(LS)	$x\in \hat{\mathcal{K}}_k$
IRCEIS	(cLS)	$x \in \hat{\mathcal{K}}_k, \ \Omega(x) = \ (L)x\ _2^2$
IRenrich	(LS)	$x \in \mathcal{K}_k + \mathcal{W}_p$
IRrrgmres	(LS)	$M=N$, $x\in \hat{\mathcal{K}}_k$
IRnnfcgls	(LS)	$x \ge 0$
IRhybrid_{lsqr}{gmres}	(cLS)	$x \in \hat{\mathcal{K}}_k$
IRhybrid_fgmres	(cLS)	$\Omega(x) = \ x\ _1$, $x \in \hat{\mathcal{K}}_k$
IRrestart	(cLS)	$x \in \mathcal{C} \cap \hat{\mathcal{K}}_k$

Introduction 000	Test problems	Iterative Solvers	Conclusior

Introduction 000	Test problems 00000	Iterative Solvers	Conclusion

Consider:

$$\min_{x\in\mathbb{R}^N}\|Ax-b\|_2^2.$$
 (LS)

Introduction		Test problems 00000	Iterative Solvers	Conclusion

Consider:

$$\min_{x\in\mathbb{R}^N}\|Ax-b\|_2^2.$$
 (LS)

A classical justification: regularization happens if

$$x_k \in \hat{\mathcal{K}}_k \,, \quad x_k \longrightarrow x^* \quad ext{when} \quad \|e\| o 0 \,.$$

Introduction	Test problems	Iterative Solvers	Conclusior
000		0000	

Consider:

$$\min_{x\in\mathbb{R}^N}\|Ax-b\|_2^2.$$
 (LS)

A classical justification: regularization happens if

>

$$x_k \in \hat{\mathcal{K}}_k \,, \quad x_k \longrightarrow x^* \quad ext{when} \quad \|e\| o 0 \,.$$

Often more can be said:

- Krylov methods "mimic" the TSVD;
- they are efficient as $\hat{\mathcal{K}}_k \simeq \hat{\mathcal{K}}_{k+1}$ for $k \ll N$.

Introduction	Test problems	Iterative Solvers	Conclusio
000		●0000	

Consider:

$$\min_{x\in\mathbb{R}^N}\|Ax-b\|_2^2.$$
 (LS)

A classical justification: regularization happens if

$$x_k \in \hat{\mathcal{K}}_k \,, \quad x_k \longrightarrow x^* \quad ext{when} \quad \|e\| o 0 \,.$$

Often more can be said:

- Krylov methods "mimic" the TSVD;
- they are efficient as $\hat{\mathcal{K}}_k \simeq \hat{\mathcal{K}}_{k+1}$ for $k \ll N$.

But sometimes this is not enough!

Introduction	Test problems	Iterative Solvers	Conclusio
000		●0000	

Consider:

$$\min_{x\in\mathbb{R}^N}\|Ax-b\|_2^2. \quad (\mathsf{LS})$$

A classical justification: regularization happens if

$$x_k \in \hat{\mathcal{K}}_k \,, \quad x_k \longrightarrow x^* \quad ext{when} \quad \|e\| o 0 \,.$$

Often more can be said:

- Krylov methods "mimic" the TSVD;
- they are efficient as $\hat{\mathcal{K}}_k \simeq \hat{\mathcal{K}}_{k+1}$ for $k \ll N$.

But sometimes this is not enough!

• "preconditioning" [Hanke and Hansen. Regularization methods for large-scale problems. Surveys Math. Industry, 1993] In the CGLS case: $x_k \in \mathcal{K}_k(L^{-1}L^{-T}A^TA, L^{-1}L^{-T}A^Tb)$

Introduction	Test problems	Iterative Solvers	Conclusio
000		●0000	

Consider:

$$\min_{x\in\mathbb{R}^N}\|Ax-b\|_2^2.$$
 (LS)

A classical justification: regularization happens if

$$x_k \in \hat{\mathcal{K}}_k \,, \quad x_k \longrightarrow x^* \quad ext{when} \quad \|e\| o 0 \,.$$

Often more can be said:

- Krylov methods "mimic" the TSVD;
- they are efficient as $\hat{\mathcal{K}}_k \simeq \hat{\mathcal{K}}_{k+1}$ for $k \ll N$.

But sometimes this is not enough!

```
• "preconditioning"
[Hanke and Hansen. Regularization methods for large-scale problems. Surveys Math. Industry, 1993]
In the CGLS case: x_k \in \mathcal{K}_k(L^{-1}L^{-T}A^TA, L^{-1}L^{-T}A^Tb)
```

enriching

[Calvetti, Reichel, and Shuibi. Enriched Krylov subspace methods for ill-posed problems. Lin. Alg. Appl., 2003] In the CGLS case: $x_k \in \mathcal{K}_k(A^T A, A^T b) \cup \mathcal{R}(W)$

Introduction	Test problems	Iterative Solvers	Conclusio
000		●0000	

Consider:

$$\min_{x\in\mathbb{R}^N}\|Ax-b\|_2^2. \quad (\mathsf{LS})$$

A classical justification: regularization happens if

>

$$x_k \in \hat{\mathcal{K}}_k \,, \quad x_k \longrightarrow x^* \quad ext{when} \quad \|e\| o 0 \,.$$

Often more can be said:

- Krylov methods "mimic" the TSVD;
- they are efficient as $\hat{\mathcal{K}}_k \simeq \hat{\mathcal{K}}_{k+1}$ for $k \ll N$.

But sometimes this is not enough!

```
• "preconditioning"
[Hanke and Hansen. Regularization methods for large-scale problems. Surveys Math. Industry, 1993]
In the CGLS case: x_k \in \mathcal{K}_k(L^{-1}L^{-T}A^TA, L^{-1}L^{-T}A^Tb)
```

enriching

[Calvetti, Reichel, and Shuibi. Enriched Krylov subspace methods for ill-posed problems. Lin. Alg. Appl., 2003] In the CGLS case: $x_k \in \mathcal{K}_k(A^T A, A^T b) \cup \mathcal{R}(W)$

nonnegativty

[G. and Wiaux. Fast nonnegative least squares through flexible Krylov subspaces, SISC, 2017]

Apply flexible CGLS to: $XA^T(Ax - b)$, $x \ge 0$.

S. Gazzola (UoB)

Test problems

Iterative Solvers

Conclusions

Interplay of regularization and projection

Introduction 000	Test problems 00000	Iterative Solvers ○●000	Conclusions
Interplay of	regularization and	l projection	
Starting from	$\min_{x\in\mathbb{R}^N}\ Ax-$	<i>b</i> ∥₂ (LS)	

Introduction 000	l est problems 00000	Iterative Solvers 0000	Conclusions
Interplay of r	egularization and	l projection	
Starting from	$\min_{x} Ax $	- <i>b</i> ₂ (LS)	

$$\min_{x \in \mathbb{R}^N} \|Ax - D\|$$

Introduction 000	Test problems 00000	Iterative Solvers 0000	Conclusions
Interplay of	regularization and	l projection	
Starting from			

$$\min_{x\in\mathbb{R}^N}\|Ax-b\|_2 \quad (\mathsf{LS})$$

consider

$$\min_{x \in \mathbb{R}^{N}} \{ \|Ax - b\|_{2}^{2} + \lambda^{2} \|x\|_{2}^{2} \} = \min_{x \in \mathbb{R}^{N}} \left\| \begin{bmatrix} A \\ \lambda I \end{bmatrix} x - \begin{bmatrix} b \\ 0 \end{bmatrix} \right\|_{2} \quad (\text{cLS})$$

Introduction 000	Test problems 00000	Iterative Solvers ●000	Conclusions
Interplay of r	egularization and	l projection	
Starting from			

$$\min_{x\in\mathbb{R}^N}\|Ax-b\|_2 \quad (\mathsf{LS})$$

consider

$$\min_{x \in \mathbb{R}^{N}} \{ \|Ax - b\|_{2}^{2} + \lambda^{2} \|x\|_{2}^{2} \} = \min_{x \in \mathbb{R}^{N}} \left\| \begin{bmatrix} A \\ \lambda I \end{bmatrix} x - \begin{bmatrix} b \\ 0 \end{bmatrix} \right\|_{2} \quad (\text{cLS})$$

• look for $x_{\lambda,k} = V_k y_{\lambda,k} \in \mathcal{V}_k \ (\mathcal{V}_k = \mathcal{R}(V_k))$ for (cLS).

Introduction 000	Test problems 00000	Iterative Solvers ••••••	Conclusions
Interplay of	regularization and	l projection	
Starting from	$\min_{x\in\mathbb{R}^N}\ Ax-$	<i>b</i> ₂ (LS)	
1 first regularia	ze, then project:		

consider

$$\min_{x \in \mathbb{R}^{N}} \{ \|Ax - b\|_{2}^{2} + \lambda^{2} \|x\|_{2}^{2} \} = \min_{x \in \mathbb{R}^{N}} \left\| \begin{bmatrix} A \\ \lambda I \end{bmatrix} x - \begin{bmatrix} b \\ 0 \end{bmatrix} \right\|_{2} \quad (cLS)$$

• look for $x_{\lambda,k} = V_k y_{\lambda,k} \in \mathcal{V}_k$ $(\mathcal{V}_k = \mathcal{R}(V_k))$ for (cLS).

2 first project, then regularize:

Introduction 000	Test problems 00000	Iterative Solvers ○●000	Conclusions
Interplay of I	regularization and	l projection	
Starting from	$\min_{x\in\mathbb{R}^N}\ Ax-$	<i>b</i> ∥₂ (LS)	

consider

$$\min_{x \in \mathbb{R}^{N}} \{ \|Ax - b\|_{2}^{2} + \lambda^{2} \|x\|_{2}^{2} \} = \min_{x \in \mathbb{R}^{N}} \left\| \begin{bmatrix} A \\ \lambda I \end{bmatrix} x - \begin{bmatrix} b \\ 0 \end{bmatrix} \right\|_{2} \quad (\text{cLS})$$

• look for $x_{\lambda,k} = V_k y_{\lambda,k} \in \mathcal{V}_k$ ($\mathcal{V}_k = \mathcal{R}(V_k)$) for (cLS).

2 first project, then regularize:

■ look for $x_k = V_k y_k \in V_k$ ($V_k = \mathcal{R}(V_k)$) approximating the solution of (LS)

 $\min_{y\in\mathbb{R}^k}\|AV_ky-b\|_2$

Introduction 000	Test problems 00000	Iterative Solvers 0000	Conclusions
Interplay of	regularization and	l projection	
Starting from	$\min_{x\in\mathbb{R}^N} \ Ax -$	<i>b</i> ∥₂ (LS)	

consider

$$\min_{x \in \mathbb{R}^{N}} \{ \|Ax - b\|_{2}^{2} + \lambda^{2} \|x\|_{2}^{2} \} = \min_{x \in \mathbb{R}^{N}} \left\| \begin{bmatrix} A \\ \lambda I \end{bmatrix} x - \begin{bmatrix} b \\ 0 \end{bmatrix} \right\|_{2} \quad (\text{cLS})$$

• look for $x_{\lambda,k} = V_k y_{\lambda,k} \in \mathcal{V}_k$ ($\mathcal{V}_k = \mathcal{R}(V_k)$) for (cLS).

2 first project, then regularize:

■ look for $x_k = V_k y_k \in V_k$ ($V_k = \mathcal{R}(V_k)$) approximating the solution of (LS)

$$\min_{y\in\mathbb{R}^k}\|AV_ky-b\|_2$$

apply some regularization

$$\min_{y \in \mathbb{R}^{k}} \left\| \begin{bmatrix} AV_{k} \\ \lambda I \end{bmatrix} y - \begin{bmatrix} b \\ 0 \end{bmatrix} \right\|_{2} \quad (\text{cLS})$$

so to get $y_{\lambda,k} \in \mathbb{R}^k$ and $x_{\lambda,k} = V_k y_{\lambda,k}$.

Introduction 000	Test problems 00000	Iterative Solvers ••••••	Conclusions
Interplay of	regularization and	projection	
Starting from	$\min_{x\in\mathbb{R}^N}\ Ax-$	$\ b\ _2$ (LS)	

consider

$$\min_{x \in \mathbb{R}^{N}} \{ \|Ax - b\|_{2}^{2} + \lambda^{2} \|x\|_{2}^{2} \} = \min_{x \in \mathbb{R}^{N}} \left\| \begin{bmatrix} A \\ \lambda I \end{bmatrix} x - \begin{bmatrix} b \\ 0 \end{bmatrix} \right\|_{2} \quad (\text{cLS})$$

• look for $x_{\lambda,k} = V_k y_{\lambda,k} \in \mathcal{V}_k$ ($\mathcal{V}_k = \mathcal{R}(V_k)$) for (cLS).

2 first project, then regularize:

■ look for $x_k = V_k y_k \in V_k$ ($V_k = \mathcal{R}(V_k)$) approximating the solution of (LS)

$$\min_{y\in\mathbb{R}^k}\|AV_ky-b\|_2$$

apply some regularization

$$\min_{y \in \mathbb{R}^{k}} \left\| \begin{bmatrix} AV_{k} \\ \lambda I \end{bmatrix} y - \begin{bmatrix} b \\ 0 \end{bmatrix} \right\|_{2} \quad (\text{cLS})$$

so to get $y_{\lambda,k} \in \mathbb{R}^k$ and $x_{\lambda,k} = V_k y_{\lambda,k}$.

These two approaches are equivalent!

S. Gazzola (UoB)
Introduction 000 Test problem

Iterative Solvers

Conclusions

The hybrid approach

Intro	du	cti	on
000			

Test problem

Iterative Solvers

The hybrid approach

The main idea:

[O'Leary and Simmons, *A bidiag.-regularization procedure for large scale ill-posed problems*, SIAM Stat.Comp., 1981] **consider additional direct regularization within the Krylov iterations**.

The hybrid approach

The main idea:

[O'Leary and Simmons, A bidiag.-regularization procedure for large scale ill-posed problems, SIAM Stat.Comp., 1981] consider additional direct regularization within the Krylov iterations.

 Generating the approximation subspace, by Arnoldi (Symmetric Lanczos), Lanczos bidiagonalization, Flexible Arnoldi algorithms:

The hybrid approach

The main idea:

[O'Leary and Simmons, A bidiag.-regularization procedure for large scale ill-posed problems, SIAM Stat.Comp., 1981] consider additional direct regularization within the Krylov iterations.

 Generating the approximation subspace, by Arnoldi (Symmetric Lanczos), Lanczos bidiagonalization, Flexible Arnoldi algorithms:

$$AV_k = Z_{k+1} \hat{C}_k \,, \quad$$
 where $\quad \widehat{C}_k \in \mathbb{R}^{(k+1) imes k}$, $\mathcal{R}(V_k) = \mathcal{K}_k$

The hybrid approach

The main idea:

[O'Leary and Simmons, A bidiag.-regularization procedure for large scale ill-posed problems, SIAM Stat.Comp., 1981] consider additional direct regularization within the Krylov iterations.

 Generating the approximation subspace, by Arnoldi (Symmetric Lanczos), Lanczos bidiagonalization, Flexible Arnoldi algorithms:

$$AV_k = Z_{k+1} \hat{\mathcal{C}}_k \,, \quad ext{where} \quad \widehat{\mathcal{C}}_k \in \mathbb{R}^{(k+1) imes k} ext{, } \mathcal{R}(V_k) = \mathcal{K}_k$$

At the *k*-th iteration:

$$\min_{y \in \mathbb{R}^k} \{ \| \hat{C}_k y - c_k \|_2^2 + \lambda_k^2 \| L_k y \|_2^2 \}$$

The hybrid approach

The main idea:

[O'Leary and Simmons, A bidiag.-regularization procedure for large scale ill-posed problems, SIAM Stat.Comp., 1981] consider additional direct regularization within the Krylov iterations.

Generating the approximation subspace, by Arnoldi (Symmetric Lanczos), Lanczos bidiagonalization, Flexible Arnoldi algorithms:

$$AV_k = Z_{k+1} \hat{C}_k$$
, where $\widehat{C}_k \in \mathbb{R}^{(k+1) imes k}$, $\mathcal{R}(V_k) = \mathcal{K}_k$

At the *k*-th iteration:

$$\min_{y \in \mathbb{R}^k} \{ \| \hat{C}_k y - c_k \|_2^2 + \lambda_k^2 \| L_k y \|_2^2 \}$$

2 Adaptively set a regularization parameter: discrepancy principle, generalized cross validation (GCV).

The hybrid approach

The main idea:

[O'Leary and Simmons, A bidiag.-regularization procedure for large scale ill-posed problems, SIAM Stat.Comp., 1981] consider additional direct regularization within the Krylov iterations.

Generating the approximation subspace, by Arnoldi (Symmetric Lanczos), Lanczos bidiagonalization, Flexible Arnoldi algorithms:

$$AV_k = Z_{k+1} \hat{C}_k$$
, where $\widehat{C}_k \in \mathbb{R}^{(k+1) imes k}$, $\mathcal{R}(V_k) = \mathcal{K}_k$

At the *k*-th iteration:

$$\min_{y \in \mathbb{R}^k} \{ \| \hat{C}_k y - c_k \|_2^2 + \lambda_k^2 \| L_k y \|_2^2 \}$$

- 2 Adaptively set a regularization parameter: discrepancy principle, generalized cross validation (GCV).
- 3 Adaptively set a regularization matrix

In	tr		С	t		

Conclusions

Parameter choice strategies for hybrid methods

Introduction		Test prol	olems		Iterative S	Solvers		
-	1.1.1.1			 	1.1.1.1.1.1.1		1.1	

Parameter choice strategies for hybrid methods

The discrepancy principle (secant update method) [G. and Novati, Automatic parameter setting for Arnoldi-Tikhonov methods, JCAM, 2014]

$$r_k(\lambda) := \|b - A x_{k,\lambda}\|_2 \leq \eta \cdot \|e\|_2, \quad \eta > 1$$

Introduction 000	Test problems	Iterative Solvers ○00●0
	• • • • • • • • • • • • • • • • • • •	

Parameter choice strategies for hybrid methods

The discrepancy principle (secant update method) [G. and Novati, Automatic parameter setting for Arnoldi-Tikhonov methods, JCAM, 2014]

$$r_k(\lambda) := \|b - A x_{k,\lambda}\|_2 \leq \eta \cdot \|e\|_2, \quad \eta > 1$$

Handling the two parameters:

$$\lambda_k^2 = \frac{\eta \|e\|_2 - r_k(0)}{r_k(\lambda_{k-1}) - r_k(0)} \lambda_{k-1}^2$$

Parameter choice strategies for hybrid methods

The discrepancy principle (secant update method)

[G. and Novati, Automatic parameter setting for Arnoldi-Tikhonov methods, JCAM, 2014]

$$r_k(\lambda) := \|b - A x_{k,\lambda}\|_2 \leq \eta \cdot \|e\|_2, \quad \eta > 1$$

Handling the two parameters:

$$\lambda_k^2 = \frac{\eta \|e\|_2 - r_k(0)}{r_k(\lambda_{k-1}) - r_k(0)} \lambda_{k-1}^2$$

Generalized cross validation (GCV)

[Chung, Nagy and O'Leary, A weighted-GCV method for Lanczos-hybrid regularization, ETNA, 2008]

$$\min_{\lambda} G(\lambda), \quad G(\lambda) = \frac{\|(I - AA_{\lambda}^{\sharp})b\|_{2}^{2}}{(\operatorname{trace}(I - AA_{\lambda}^{\sharp}))^{2}}$$

Introduction 000	Test problems 00000	Iterative Solvers	Conclu
D I .	and the second	Contraction of the	

Regularization matrix choice for hybrid methods

A notable example: enforcing sparsity (ℓ_1 -norm penalization):

Introduction 000	Test problems 00000	Iterative Solvers	Conclusio
Regularization	matrix choice for	or hybrid methods	

$$\min_{x} \left\{ \|Ax - b\|_{2}^{2} + \lambda^{2} \|x\|_{1} \right\}, \quad A \in \mathbb{R}^{N \times N}.$$

Introduction 000	Test problems 00000	Iterative Solvers	Conclusion
Regularization	matrix choice	for hybrid methods	

$$\min_{x} \left\{ \|Ax - b\|_{2}^{2} + \lambda^{2} \|x\|_{1} \right\}, \quad A \in \mathbb{R}^{N \times N}.$$

With an iteratively reweighted-norm approach:

$$\|x\|_1 pprox \|\mathcal{W}x\|_2^2 = \|\mathcal{W}_m x\|_2^2, \quad ext{with} \quad \mathcal{W}_m = L_m = ext{diag}\left(rac{1}{\sqrt{|x_{m-1}|}}
ight).$$

Introduction 000	Test problems 00000	Iterative Solvers	Conclusion
Regularization	matrix choice	for hybrid methods	

$$\min_{x} \left\{ \|Ax - b\|_{2}^{2} + \lambda^{2} \|x\|_{1} \right\}, \quad A \in \mathbb{R}^{N \times N}.$$

With an iteratively reweighted-norm approach:

$$\|x\|_1 pprox \|\mathcal{W}x\|_2^2 = \|\mathcal{W}_m x\|_2^2, \quad ext{with} \quad \mathcal{W}_m = L_m = ext{diag}\left(rac{1}{\sqrt{|x_{m-1}|}}
ight).$$

$$\min_{x} \left\{ \|b - Ax\|_{2}^{2} + \lambda \|L_{m}(x - x^{*})\|_{2}^{2} \right\}$$

Introduction 000	Test problems 00000	Iterative Solvers	Conclusion
Regularization	matrix choice	for hybrid methods	

$$\min_{x} \left\{ \|Ax - b\|_{2}^{2} + \lambda^{2} \|x\|_{1} \right\}, \quad A \in \mathbb{R}^{N \times N}.$$

With an iteratively reweighted-norm approach:

$$\|x\|_1 pprox \|\mathcal{W}x\|_2^2 = \|\mathcal{W}_m x\|_2^2, \quad ext{with} \quad \mathcal{W}_m = L_m = ext{diag}\left(rac{1}{\sqrt{|x_{m-1}|}}
ight)\,.$$

Consider a standard form transformation

$$\begin{split} \min_{x} \left\{ \|b - Ax\|_{2}^{2} + \lambda \|L_{m}(x - x^{*})\|_{2}^{2} \right\} & \qquad \widetilde{A}_{m} = AL_{m}^{-1} \\ \min_{\widetilde{x}} \{\|b - \widetilde{A}_{m}\widetilde{x}\|_{2}^{2} + \widetilde{\lambda} \|\widetilde{x} - \widetilde{x}^{*}\|_{2}^{2} \} & \qquad \widetilde{x}^{*} = L_{m}x^{*} \\ & \qquad \widetilde{x} = L_{m}x \end{split}$$

Introduction 000	Test problems	Iterative Solvers	Conclusion
Regularization	matrix choice	for hybrid methods	

$$\min_{x} \left\{ \|Ax - b\|_{2}^{2} + \lambda^{2} \|x\|_{1} \right\}, \quad A \in \mathbb{R}^{N \times N}.$$

With an iteratively reweighted-norm approach:

$$\|x\|_1 pprox \|\mathcal{W}x\|_2^2 = \|\mathcal{W}_m x\|_2^2, \quad ext{with} \quad \mathcal{W}_m = L_m = ext{diag}\left(rac{1}{\sqrt{|x_{m-1}|}}
ight)\,.$$

Consider a standard form transformation

$$\begin{split} \min_{x} \left\{ \|b - Ax\|_{2}^{2} + \lambda \|L_{m}(x - x^{*})\|_{2}^{2} \right\} & \qquad \widetilde{A}_{m} = AL_{m}^{-1} \\ \min_{x} \{\|b - \widetilde{A}_{m}\widetilde{x}\|_{2}^{2} + \widetilde{\lambda}\|\widetilde{x} - \widetilde{x}^{*}\|_{2}^{2} \} \\ & \qquad \widetilde{x}^{*} = L_{m}x^{*} \\ & \qquad \widetilde{x} = L_{m}x \end{split}$$
Efficiently handled by Flexible Arnoldi, in a hybrid fashion.

[G. and Nagy, Generalized AT method for sparse reconstruction, SISC, 2014]

Introduction 000	Test problems 00000	Iterative Solvers	Conclusion
Regularization	matrix choic	e for hybrid methods	

$$\min_{x} \left\{ \|Ax - b\|_{2}^{2} + \lambda^{2} \|x\|_{1} \right\}, \quad A \in \mathbb{R}^{N \times N}.$$

With an iteratively reweighted-norm approach:

$$\|x\|_1 pprox \|\mathcal{W}x\|_2^2 = \|\mathcal{W}_m x\|_2^2, \quad ext{with} \quad \mathcal{W}_m = L_m = ext{diag}\left(rac{1}{\sqrt{|x_{m-1}|}}
ight)\,.$$

Consider a standard form transformation

$$\min_{x} \left\{ \|b - Ax\|_{2}^{2} + \lambda \|L_{m}(x - x^{*})\|_{2}^{2} \right\}$$

$$\min_{\widetilde{u}}\{\|\boldsymbol{b}-\widetilde{A}_m\widetilde{x}\|_2^2+\widetilde{\lambda}\|\widetilde{x}-\widetilde{x}^*\|_2^2\}$$

 $\widetilde{A}_m = AL_m^{-1}$ $\widetilde{X}^* = L_m X^*$ $\widetilde{X} = L_m X$

Efficiently handled by Flexible Arnoldi, in a hybrid fashion. [G. and Nagy, Generalized AT method for sparse reconstruction, SISC, 2014]

Other possible approaches: restarted Krylov methods.

Introduction	Test problems	Iterative Solvers	Conclusions
000	00000	00000	
Wrapping up			

Introduction	Test problems	Iterative Solvers	Conclusions
000	00000	00000	
Wrapping up			

"new" iterative solvers...

Introduction	Test problems	Iterative Solvers	Conclusions
000	00000	00000	
Wrapping up			

"new" iterative solvers...much more to explore (and to code!)

Introduction 000	Test problems 00000	Iterative Solvers	Conclusions
Wrapping up			

- "new" iterative solvers...much more to explore (and to code!)
- "new" test problems...

Introduction 000	Test problems 00000	Iterative Solvers	Conclusions
Wrapping up			

- "new" iterative solvers...much more to explore (and to code!)
- "new" test problems...much more to explore (and to code!)

Introduction	Test problems	Iterative Solvers	Conclusions
000	00000	00000	
Wrapping up			

- "new" iterative solvers...much more to explore (and to code!)
- "new" test problems...much more to explore (and to code!)

Some references:



P. C. Hansen.

Discrete Inverse Problems: Insight and Algorithms. SIAM, 2010.



S. Gazzola, P. Novati, and M. R. Russo.

On Krylov projection methods and Tikhonov regularization. ETNA, 2015.

Introduction	Test problems	Iterative Solvers	Conclusions
000	00000	00000	
Wrapping up			

- "new" iterative solvers...much more to explore (and to code!)
- "new" test problems...much more to explore (and to code!)

Some references:



P. C. Hansen.

Discrete Inverse Problems: Insight and Algorithms. SIAM, 2010.



S. Gazzola, P. Novati, and M. R. Russo.

On Krylov projection methods and Tikhonov regularization. ETNA, 2015.

THANKS FOR YOUR ATTENTION!