Numerical Methods for Large-Scale Ill-Posed Inverse Problems

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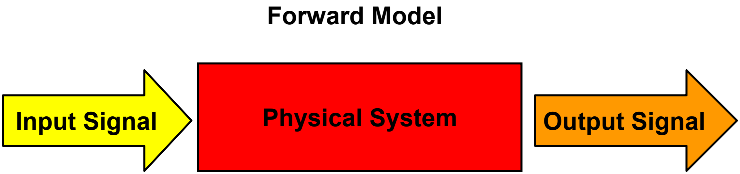
Dianne O'Leary (University of Maryland)
Ioannis Sechopoulos (Emory)
Chao Yang (Lawrence Berkeley National Laboratory)

What is an inverse problem?



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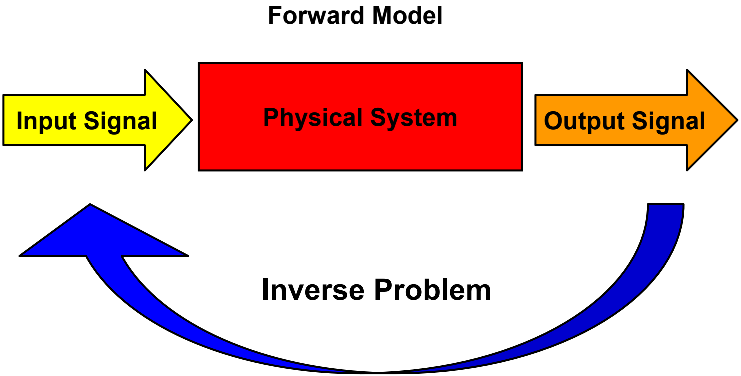

Application: Image Deblurring

- Given: Blurred image and some information about the blurring
- Goal: Compute approximation of true image

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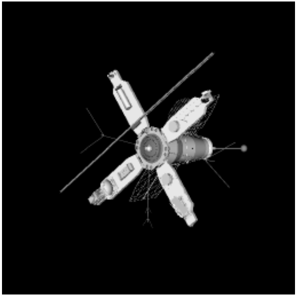
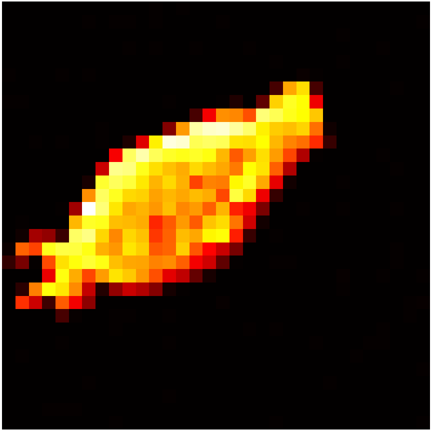


Application: Super-Resolution Imaging

- Given: LR images and some information about the motion parameters

1−th low resolution image



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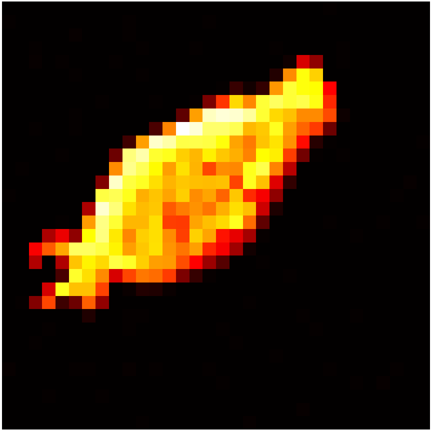
8−th low resolution image



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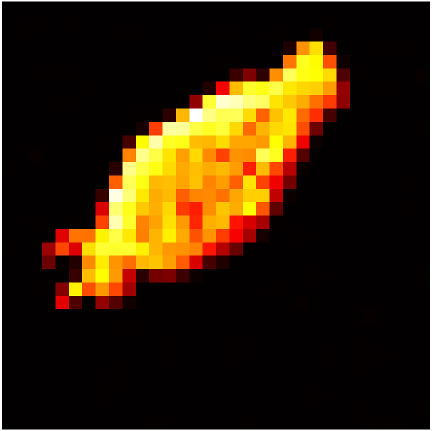
- Given: LR images and some information about the motion parameters

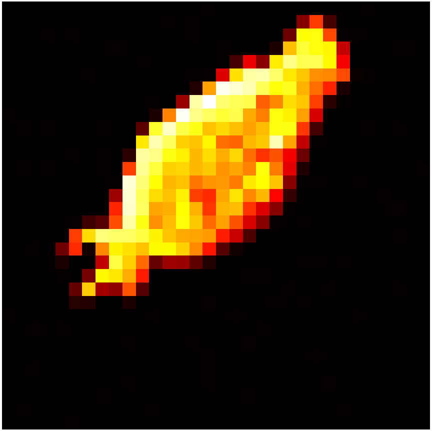
15−th low resolution image



Application: Super-Resolution Imaging

- Given: LR images and some information about the motion parameters

22−th low resolution image



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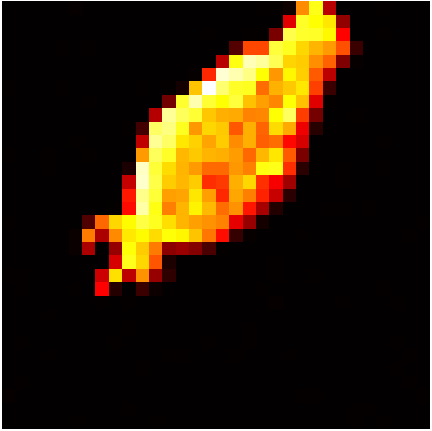
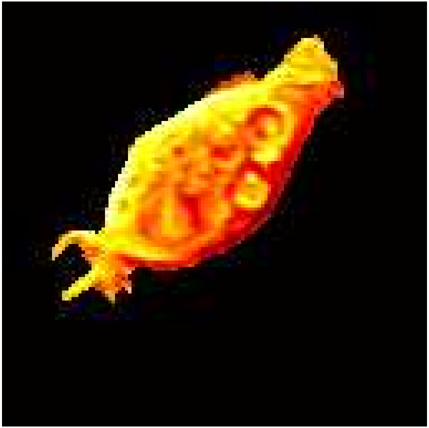
29−th low resolution image



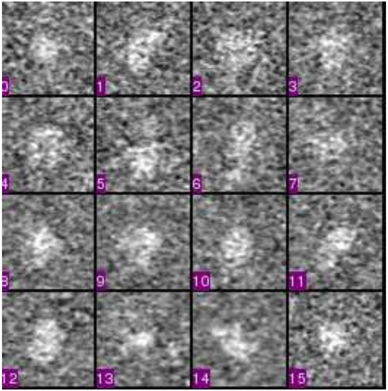
Application: Super-Resolution Imaging

- Given: LR images and some information about the motion parameters
- Goal: Improve parameters and approximate HR image



Application: Tomographic Imaging

- Given: 2D projection images
- Goal: Approximate 3D volume



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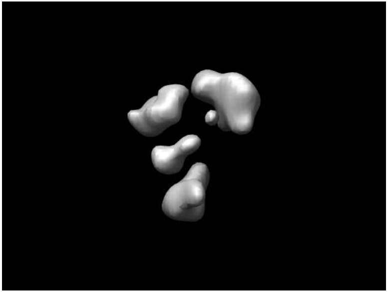

What is an Ill-Posed Inverse Problem?

Hadamard (1923): A problem is ill-posed if the solution

- does not exist,
- is not unique, or
- does not depend continuously on the data.

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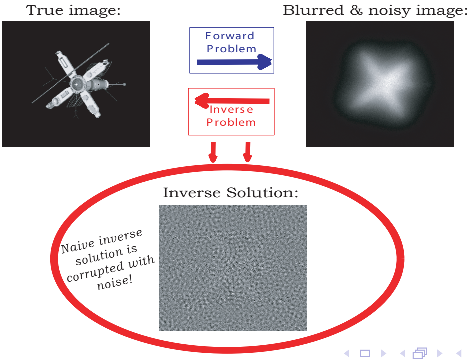

Outline

1. Regularization for Least Squares Systems
2. High Performance Implementation
3. Polyenergetic Tomosynthesis
4. Concluding Remarks

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1. Regularization for Least Squares Systems
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3. Polyenergetic Tomosynthesis
4. Concluding Remarks

The Linear Problem

$$\mathbf{b} = \mathbf{A}\mathbf{x} + \varepsilon$$

where

- $\mathbf{x} \in \mathcal{R}^n$ - true data
- $\mathbf{A} \in \mathcal{R}^{m \times n}$ - large, ill-conditioned matrix
- $\varepsilon \in \mathcal{R}^m$ - noise, statistical properties may be known
- $\mathbf{b} \in \mathcal{R}^m$ - known, observed data

Goal: Given **b** and **A**, compute approximation of **x**

Regularization

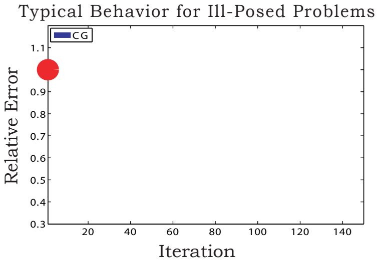
Tikhonov Regularization

$$\min_{\mathbf{x}} \left\{ ||\mathbf{b} - \mathbf{A}\mathbf{x}||_2^2 + \lambda^2 ||\mathbf{L}\mathbf{x}||_2^2 \right\} \quad \Leftrightarrow \quad \min_{\mathbf{x}} \left\| \begin{bmatrix} \mathbf{b} \\ \mathbf{0} \end{bmatrix} - \begin{bmatrix} \mathbf{A} \\ \lambda \mathbf{L} \end{bmatrix} \mathbf{x} \right\|_2$$

- Selecting a good regularization parameter, λ, is difficult
  - Discrepancy Principle
  - Generalized Cross-Validation
  - L-curve
- Difficult for large-scale problems

Illustration of Semi-convergence Behavior

$$\min_{\mathbf{x}} \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_2$$



Iteration 0

Illustration of Semi-convergence Behavior

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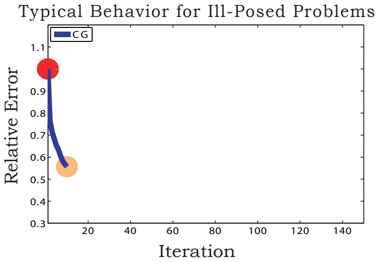

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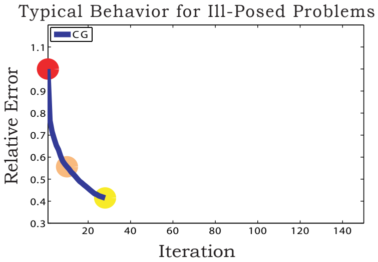


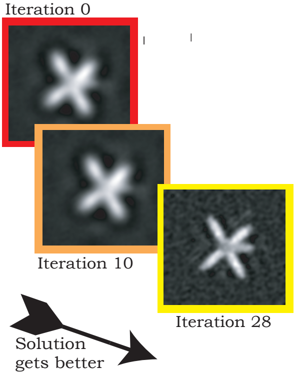
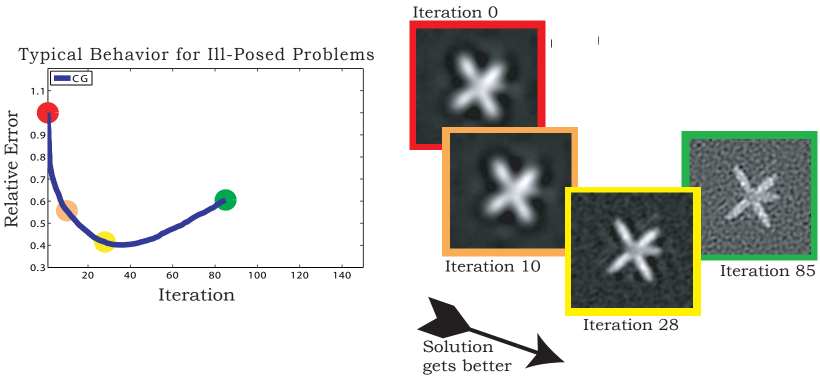


Illustration of Semi-convergence Behavior

$$\min_{\mathbf{x}} \|\mathbf{b} - \mathbf{Ax}\|_2$$



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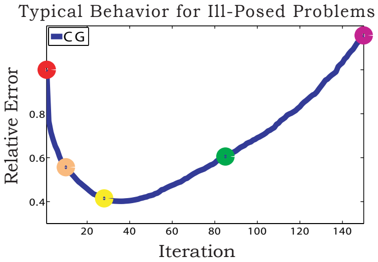

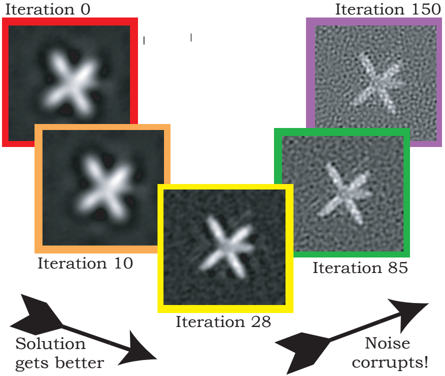

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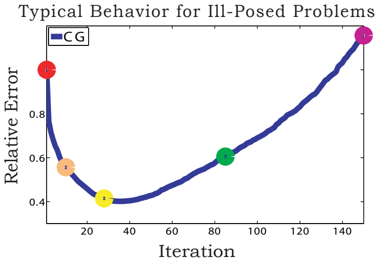
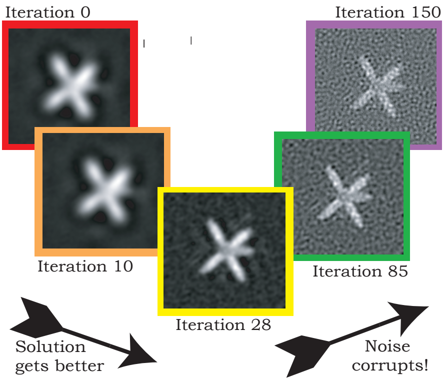
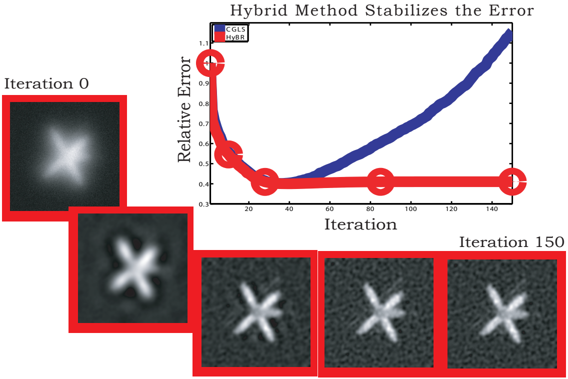




Either find a good stopping criteria or ...

Motivation to use a Hybrid Method

... avoid semi-convergence behavior altogether!



Previous Work on Hybrid Methods

Regularization embedded in iterative method:

- O'Leary and Simmons, SISSC, 1981.
- Björck, BIT 1988.
- Björck, Grimme, and Van Dooren, BIT, 1994.
- Larsen, PhD Thesis, 1998.
- Hanke, BIT 2001.
- Kilmer and O'Leary, SIMAX, 2001.
- Kilmer, Hansen, Espanol, 2006.

Use iterative method to solve regularized problem:

- Golub, Von Matt, Numer. Math.,1991
- Calvetti, Golub, Reichel, BIT, 1999
- Frommer, Maass , SISC, 1999

Lanczos Bidiagonalization(LBD)

Given **A** and **b**, for $k = 1, 2, ...,$ compute

- $\mathbf{W} = \begin{bmatrix} \mathbf{w}_1 & \mathbf{w}_2 & \cdots & \mathbf{w}_k & \mathbf{w}_{k+1} \end{bmatrix}, \quad \mathbf{w}_1 = \mathbf{b}/||\mathbf{b}||$
- $\mathbf{Y} = \begin{bmatrix} \mathbf{y}_1 & \mathbf{y}_2 & \cdots & \mathbf{y}_k \end{bmatrix}$
- $\mathbf{B} = \begin{bmatrix} \alpha_1 & & & \\ \beta_2 & \alpha_2 & & \\ & \ddots & \ddots & \\ & & \beta_k & \alpha_k \\ & & & \beta_{k+1} \end{bmatrix}$

where **W** and **Y** have orthonormal columns, and

$$\mathbf{AY} = \mathbf{WB}$$

The Projected Problem

After k steps of LBD, we solve the *projected* LS problem:

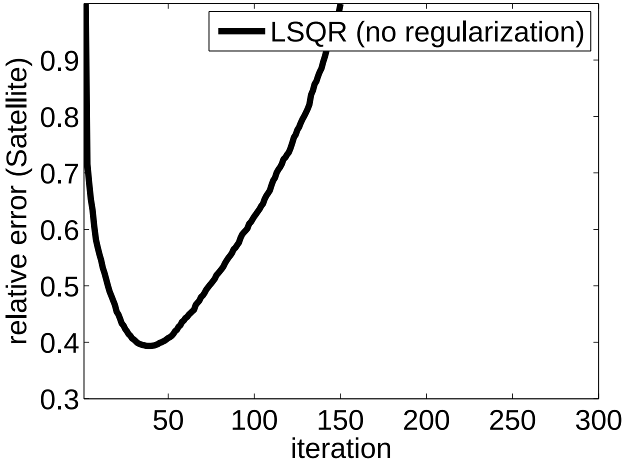
$$\min_{\mathbf{x} \in R(\mathbf{Y})} ||\mathbf{b} - \mathbf{A}\mathbf{x}||_2 = \min_{\mathbf{f}} ||\mathbf{W}^T\mathbf{b} - \mathbf{B}\mathbf{f}||_2$$

where $\mathbf{x} = \mathbf{Y}\mathbf{f}$.

Remarks:

- Ill-posed problem $\Rightarrow$ **B** may be very ill-conditioned.
- **B** is much smaller than **A**
- Standard techniques (e.g. GCV) to find λ and stopping point

Lanczos Hybrid Method in Action: Satellite



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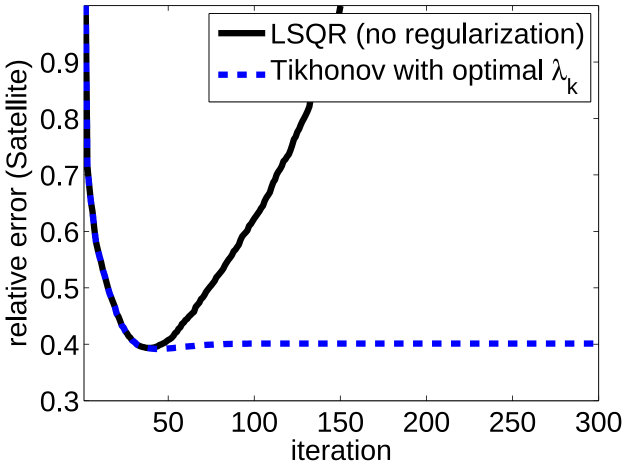

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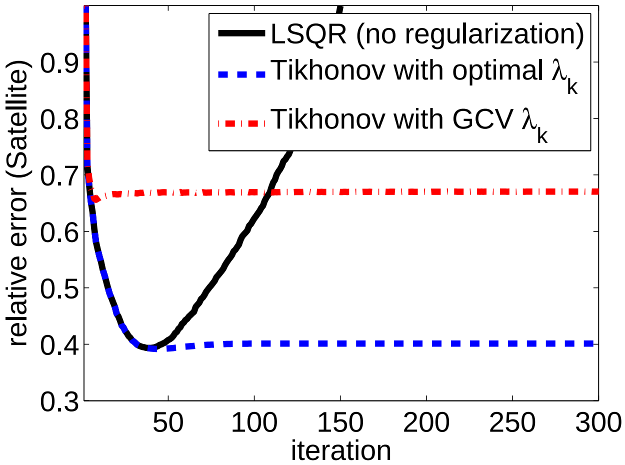


A Novel Approach: Weighted GCV

$$\min_{\mathbf{f}} ||\mathbf{W}^T\mathbf{b} - \mathbf{B}\mathbf{f}||_2$$

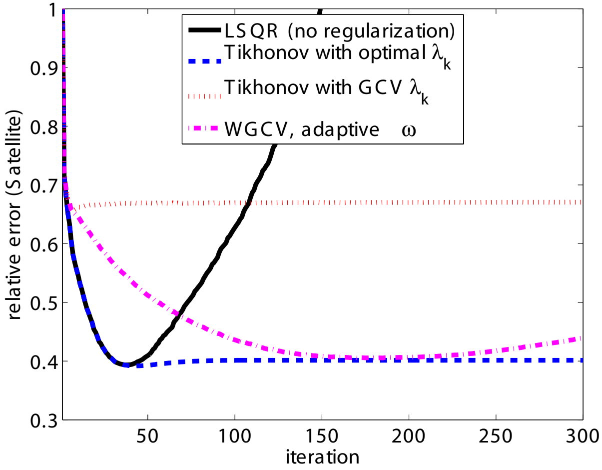
GCV tends to over smooth, use weighted GCV function with $\omega < 1$:

$$G(\omega, \lambda) = \frac{n||(I - \mathbf{B}\mathbf{B}_\lambda^\dagger)\mathbf{W}^T\mathbf{b}||^2}{\left[\text{trace}(I - \omega\mathbf{B}\mathbf{B}_\lambda^\dagger)\right]^2}$$

New adaptive approach to select ω
MATLAB implementation:

$$>> \mathbf{x} = HyBR(\mathbf{A}, \mathbf{b});$$

Results for Satellite



The Nonlinear Problem

$$\mathbf{b} = \mathbf{A}(\mathbf{y})\mathbf{x} + \varepsilon$$

where

$\mathbf{x}$ - true data

$\mathbf{A}(\mathbf{y})$ - large, ill-conditioned matrix defined by parameters $\mathbf{y}$ (registration, blur, etc.)

ε - additive noise

$\mathbf{b}$ - known, observed data

Goal: Approximate $\mathbf{x}$ and improve parameters $\mathbf{y}$

Mathematical Representation

- We want to find **x** and **y** so that

$$\mathbf{b} = \mathbf{A}(\mathbf{y})\mathbf{x} + \mathbf{e}$$

- With Tikhonov regularization, solve

$$\min_{\mathbf{x},\mathbf{y}} \left\| \begin{bmatrix} \mathbf{A}(\mathbf{y}) \\ \lambda \mathbf{I} \end{bmatrix} \mathbf{x} - \begin{bmatrix} \mathbf{b} \\ \mathbf{0} \end{bmatrix} \right\|_2^2$$

Some Considerations:

- Problem is linear in **x**, nonlinear in **y**.
- $\mathbf{y} \in \mathcal{R}^p$, $\mathbf{x} \in \mathcal{R}^n$, with $p \ll n$.

Separable Nonlinear Least Squares

Variable Projection Method:

- Implicitly eliminate linear term.
- Optimize over nonlinear term.

Some general references:

Golub and Pereyra, SINUM 1973 (also IP 2003)
Kaufman, BIT 1975
Osborne, SINUM 1975 (also ETNA 2007)
Ruhe and Wedin, SIREV, 1980

Variable Projection Method

Instead of optimizing over both **x** and **y**:

$$\min_{\mathbf{x},\mathbf{y}} \phi(\mathbf{x},\mathbf{y}) = \min_{\mathbf{x},\mathbf{y}} \left\| \begin{bmatrix} \mathbf{A}(\mathbf{y}) \\ \lambda \mathbf{I} \end{bmatrix} \mathbf{x} - \begin{bmatrix} \mathbf{b} \\ \mathbf{0} \end{bmatrix} \right\|_2^2$$

Minimize the reduced cost functional:

$$\min_{\mathbf{y}} \psi(\mathbf{y}), \quad \psi(\mathbf{y}) = \phi(\mathbf{x}(\mathbf{y}),\mathbf{y})$$

where $\mathbf{x}(\mathbf{y})$ is the solution of

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Gauss-Newton Algorithm

choose initial $\mathbf{y}_0$

for $k = 0, 1, 2, \ldots$

$$\mathbf{x}_k = \arg\min_{\mathbf{x}} \left\| \begin{bmatrix} \mathbf{A}(\mathbf{y}_k) \\ \lambda_k \mathbf{I} \end{bmatrix} \mathbf{x} - \begin{bmatrix} \mathbf{b} \\ \mathbf{0} \end{bmatrix} \right\|_2$$

$$\mathbf{r}_k = \mathbf{b} - \mathbf{A}(\mathbf{y}_k)\,\mathbf{x}_k$$

$$\mathbf{d}_k = \arg\min_{\mathbf{d}} \|\mathbf{J}_\psi \mathbf{d} - \mathbf{r}_k\|_2$$

$$\mathbf{y}_{k+1} = \mathbf{y}_k + \mathbf{d}_k$$

end

Gauss-Newton Algorithm with HyBR

choose initial $\mathbf{y}_0$

for $k = 0, 1, 2, \ldots$

$$\mathbf{x}_k = \arg\min_{\mathbf{x}} \left\| \begin{bmatrix} \mathbf{A}(\mathbf{y}_k) \\ \lambda_k \mathbf{I} \end{bmatrix} \mathbf{x} - \begin{bmatrix} \mathbf{b} \\ \mathbf{0} \end{bmatrix} \right\|_2 \quad \Rightarrow \mathbf{x}_k = \text{HyBR}(\mathbf{A}(\mathbf{y}_k), \mathbf{b})$$

$$\mathbf{r}_k = \mathbf{b} - \mathbf{A}(\mathbf{y}_k)\,\mathbf{x}_k$$

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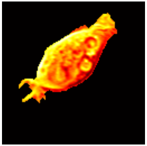
end

Numerical Results: Super-resolution

Inverse Problem

Given:

Goal:



Gauss-Newton Iterations

	Error of $\mathbf{y}_k$	λ_k
0	0.5810	0.2519
1	0.3887	0.2063
2	0.2495	0.1765
3	0.1546	0.1476
4	0.1077	0.1254
5	0.0862	0.1139
6	0.0763	0.1102
7	0.0706	0.1077
8	0.0667	0.1067

Reconstructed Image

Numerical Results: Super-resolution

Inverse Problem

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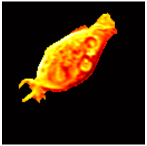
Goal:



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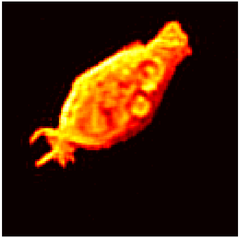

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Mathematical Model

$$\min_{\mathbf{x}} \frac{1}{2}||\mathbf{A}\mathbf{x} - \mathbf{b}||^2$$

where

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_1 \\ \vdots \\ \mathbf{A}_m \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} \mathbf{b}_1 \\ \vdots \\ \mathbf{b}_m \end{bmatrix}$$

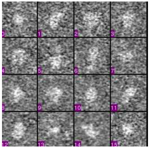
Some Applications:

- Super-resolution
- Tomography - Cryo-Electron Microscopy

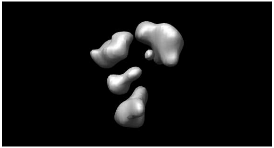
An Application: Cryo-EM

Inverse Problem

Given:



Goal:



$$\min_{\mathbf{x}} \rho(\mathbf{x}) = \frac{1}{2} \sum_{i=1}^{m} ||\mathbf{A}_i \mathbf{x} - \mathbf{b}_i||^2$$

where

- $\mathbf{x} \in \mathcal{R}^{n^3}$ represents the 3-D electron density map
- $\mathbf{b}_i \in \mathcal{R}^{n^2} (i = 1, 2, ..., m)$ represents 2-D projection images
- $\mathbf{A}_i = \mathbf{A}(\mathbf{y}_i) \in \mathcal{R}^{n^2 \times n^3}$ represents projection
  - $\mathbf{y}_i$ - translation parameters and Euler angles

An Application: Cryo-EM

Inverse Problem

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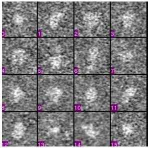

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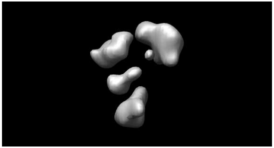

$$\min_{\mathbf{x}} \rho(\mathbf{x}) \equiv \frac{1}{2}\sum_{i=1}^{m} ||\mathbf{A}_i\mathbf{x} - \mathbf{b}_i||^2$$

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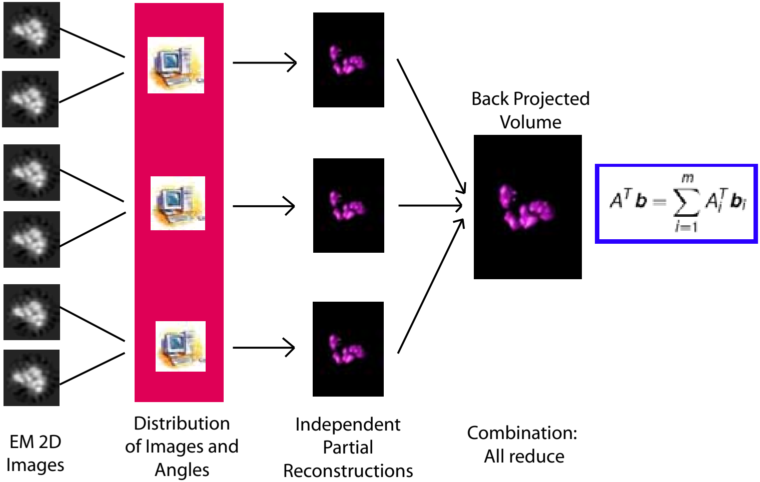
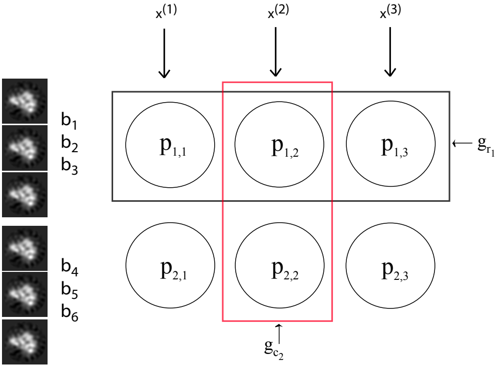
Parallelization using 1D data distribution



New Parallelization using 2D data distribution

- Distribute images along rows.
- Distribute volume along columns.



Forward and Back Projection on 2D Topology

$$\mathbf{A}_i = \begin{bmatrix} \mathbf{A}_i^{(1)} & \mathbf{A}_i^{(2)} & \cdots & \mathbf{A}_i^{(n_c)} \end{bmatrix}, \quad \mathbf{x} = \begin{bmatrix} \mathbf{x}^{(1)} \\ \mathbf{x}^{(2)} \\ \vdots \\ \mathbf{x}^{(n_c)} \end{bmatrix}, \nabla\rho = \begin{bmatrix} \nabla\rho_{\mathbf{x}^{(1)}} \\ \nabla\rho_{\mathbf{x}^{(2)}} \\ \vdots \\ \nabla\rho_{\mathbf{x}^{(n_c)}} \end{bmatrix}$$

$$\mathbf{A}_i\mathbf{x} = \sum_{j=1}^{n_c} \mathbf{A}_i^{(j)}\mathbf{x}^{(j)} \quad \Rightarrow \quad \text{All Reduce along Rows}$$

$$\nabla\rho_{\mathbf{x}^{(j)}} = \sum_{i=1}^{m} (\mathbf{A}_i^{(j)})^T \mathbf{r}_{(i)} \quad \Rightarrow \quad \text{All Reduce along Columns}$$

New MPI Parallel Performance

- Good for very large problems
- Adenovirus Data Set: 500 × 500 pixels, 959 (×60) images

n_r	n_c	Wall clock seconds	speedup
137	7	9635	1
959	2	4841	2
959	4	2406	4
959	8	1335	7.2
959	16	609	15.8

- SPARX software package

Outline

1. Regularization for Least Squares Systems
2. High Performance Implementation
3. Polyenergetic Tomosynthesis
4. Concluding Remarks

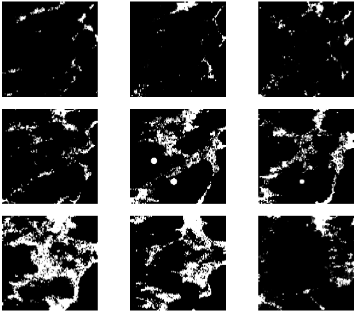
Digital Tomosynthesis

- X-ray Mammography
- Digital Tomosynthesis
- Computed Tomography

An Inverse Problem

- Given: 2D projection images
- Goal: Reconstruct a 3D volume

True Images

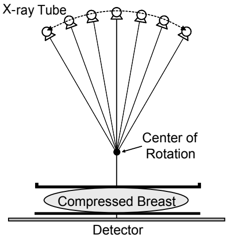


Simulated Problem

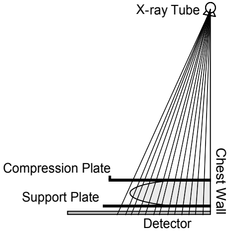
Original object:
$300 \times 300 \times 200$ voxels
($7.5 \times 7.5 \times 5$ cm)

21 projection images:
200×300 pixels
(10×15 cm)
-30° to 30°, every 3°

Reconstruction:
$150 \times 150 \times 50$ voxels
($7.5 \times 7.5 \times 5$ cm)



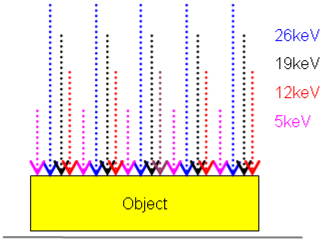
Front view



Side view with X-ray tube at 0°

Polyenergetic Model

- Incident X-ray has a distribution of energies
- 43 energy levels: 5keV - 26keV



Consequences:

- Beam Hardening: Low energy photons preferentially absorbed
- Unnecessary radiation
- Linear attenuation coefficient depends on energy

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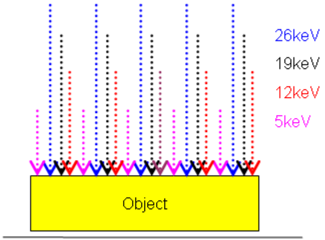

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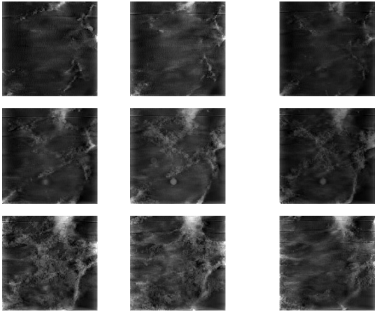
Monoenergetic Algorithm

- Lange and Fessler's Convex MLEM Algorithm
- Beam hardening artifacts

Monoenergetic Reconstruction



Previous Methods

Methods for eliminating beam hardening artifacts:

- Dual Energy Methods

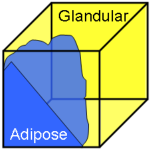
  Alvarez and Macovski (1976), Fessler et al (2002)
- FBP + Segmentation

  Joseph and Spital (1978)
- Filter function based on density

  De Man et al (2001), Elbakri and Fessler (2003)

A Polyenergetic Mathematical Representation

Voxel j



Energy-dependent Attenuation Coefficient:

$$\mu(e)^{(j)} = s(e)x^{(j)} + z(e)$$

where

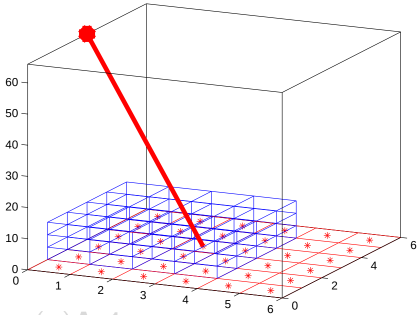
$x^{(j)}$ represents unknown glandular fraction of j^{th} voxel

$s(e)$ and $z(e)$ are known linear fit coefficients

Computing Image Projections

- Ray Trace:

$$\int_{L_i} \mu(e) dl \approx \sum_{j=1}^{N} \mu(e)^{(j)} a^{(ij)}$$



- Vector Notation

$$\mu(e) = s(e)\mathbf{x} + z(e) \quad \Rightarrow \quad s(e)\mathbf{A}_\theta \mathbf{x} + z(e)\mathbf{A}_\theta \mathbf{1}$$

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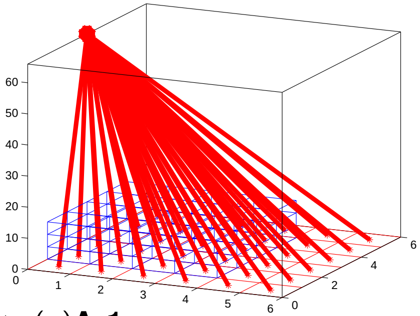

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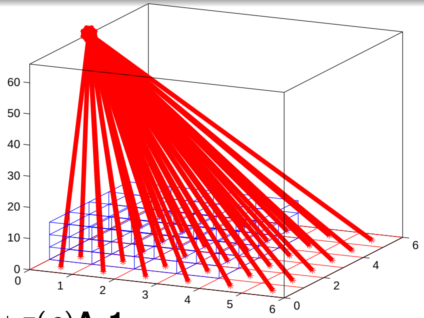

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Polyenergetic Projection:

$$\sum_{e=1}^{n_e} \varrho(e) \exp\left(-[s(e)\mathbf{A}_\theta\mathbf{x}_{true} + z(e)\mathbf{A}_\theta\mathbf{1}]\right)$$

Statistical Model

Given **x**, define for pixel *i* the expected value:

$$\bar{b}_\theta^{(i)} = \sum_{e=1}^{n_e} \varrho(e) \exp\left(-[s(e)\mathbf{A}_\theta \mathbf{x} + z(e)\mathbf{A}_\theta \mathbf{1}]\right).$$

Let $\bar{\eta}^{(i)}$ be the statistical mean of the noise.

Then $\bar{b}_\theta^{(i)} + \bar{\eta}^{(i)} \in \mathcal{R}$ is the expected or average observation.

Observed Data: $b_\theta^{(i)} \sim \text{Poisson}(\bar{b}_\theta^{(i)} + \bar{\eta}^{(i)})$

Statistical Model

Likelihood Function:

$$p(\mathbf{b}_\theta, \mathbf{x}) = \prod_{i=1}^{M} \frac{e^{-(\bar{b}_\theta^{(i)} + \bar{\eta}^{(i)})} (\bar{b}_\theta^{(i)} + \bar{\eta}^{(i)})^{b_\theta^{(i)}}}{b_\theta^{(i)}!}$$

Negative Log Likelihood Function:

$$\begin{aligned} -L_\theta(\mathbf{x}) &= -\log p(\mathbf{b}_\theta, \mathbf{x}) \\ &= \sum_{i=1}^{M} (\bar{b}_\theta^{(i)} + \bar{\eta}^{(i)}) - b_\theta^{(i)} \log(\bar{b}_\theta^{(i)} + \bar{\eta}^{(i)}) \end{aligned}$$

Volume Reconstruction

Maximum Likelihood Estimate:

$$\mathbf{x}_{MLE} = \underset{\mathbf{x}}{\text{argmin}} \left\{ \sum_{\theta=1}^{n_\theta} -L_\theta(\mathbf{x}) \right\}$$

Numerical Optimization:

- Gradient Descent:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha_k \nabla L(\mathbf{x}_k), \quad \text{where} \quad \nabla L(\mathbf{x}_k) = \mathbf{A}^T \mathbf{v}_k$$

- Newton Approach:

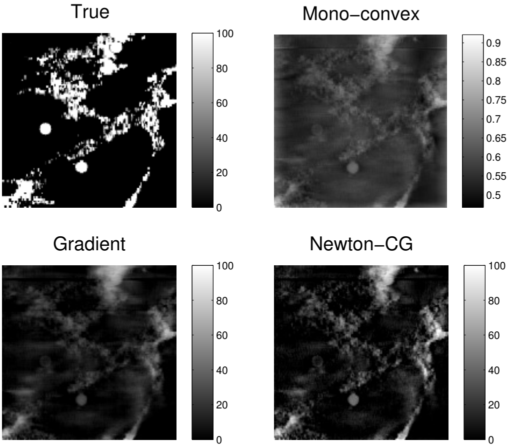
$$\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha_k \mathbf{H}_k^{-1} \nabla L(\mathbf{x}_k), \quad \text{where} \quad \mathbf{H}_k = \mathbf{A}^T \mathbf{W}_k \mathbf{A}$$

Numerical Results

- Initial guess: 50% glandular tissue
- Newton-CG inner stopping criteria:
  - Max 50 inner iterations
  - residual tolerance < 0.1

Gradient Descent		Newton Iteration		
Iteration	Relative Error	Iteration	Relative Error	CG Iterations
0	1.7691	0	1.7691	-
1	1.0958	1	1.1045	3
5	0.8752	2	0.8630	2
10	0.8320	3	0.8403	2
25	0.8024	4	0.7925	16

Compare Images



Some Considerations

- Convexity

  Severe nonlinearities $\Rightarrow$ Cost function is not convex

- Regularization

$$\mathbf{x}_{MAP} = \underset{\mathbf{x}}{\operatorname{argmin}}\{-L(\mathbf{x}) + \lambda \mathbf{R}(\mathbf{x})\}$$

  - Need good regularizer, $\mathbf{R}(\mathbf{x})$:

    Huber penalty, Markov Random Fields, Total Variation

  - Need good methods for choosing λ

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Concluding Remarks

- Inverse problems arise in many imaging applications.
- Hybrid methods:
  - efficient solvers for large scale LS problems
  - effective linear solvers for nonlinear problems
- Separable nonlinear LS models exploit high level structure
- High performance implementation allows reconstruction of large volumes with high resolution
- Polyenergetic tomosynthesis:
  - Novel mathematical framework
  - Standard optimization made feasible
  - Better reconstructed images

References

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  - Chung, Nagy, O'Leary. ETNA (2008)
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Thank you!