ADVANCED RECONSTRUCTION FOR ELECTRON MICROSCOPY

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OUTLINE

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1. **OVERVIEW OF MBIR**

\[
(\hat{x}, \hat{\phi}) \leftarrow \text{arg max}_{x, \phi} \left\{ p(x, \phi | y) \right\} = \text{arg min}_{x, \phi} \left\{ -\log p(y | x, \phi) - \log p(x) \right\}
\]

1. \( p(y | x, \phi) \): Likelihood
2. \( p(x) \): Prior Model

\[\phi\]
\[p(.)\]: Probability density function

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Iteratively update the parameters to minimize a cost function.
2. **PREVIOUS WORK**

The next few slides pertaining to the previous work are courtesy of S. V. Venkatakrishnan (Venkat) who sends his
MBIR FOR HAADF-STEM TOMOGRAPHY*

- Polystyrene functionalized titanium dioxide nanoparticles**
- 87 tilts from -70° to +70°

MBIR FOR BF-(S)TEM TOMOGRAPHY*

- Aluminum nanoparticles in a carbon matrix
- 36 tilts from -70° to +70°

MBIR FOR LOW-DOSE TOMOGRAPHY*

- Ferritin – protein used for iron storage
- Sample degrades when exposed to a high electron-dose

Data at zero tilt

3. LEADING TO ADVANCED PRIOR MODELS

- MBIR for tomography – use of “simple” Markov Random Field priors.

- Using advanced image models – enable improved reconstruction quality/ reduce data collected.

- Can reduce collection times and sample damage for bio-imaging.
CHALLENGES INVOLVED IN ADVANCED PRIOR MODELING

• Choice of prior effects choice of optimization algorithm for MBIR – tight coupling of forward and prior model.

• Tremendous progress in simple inverse problem – denoising - using advanced “priors” based on non-local similarities in images.

• But we have no clear algorithmic framework to use these advanced denoising techniques in applications like tomography.
SOLUTION: PLUG-AND-PLAY PRIORS

\[ y : \text{Data} \]

\[ \hat{v} - u \]

\[ \hat{x} \]

\[ \hat{x} + u \]

\[ \lambda : \text{Forward model regularization parameter} \]

\[ \beta : \text{Denoising parameter} \]

Invert based on forward model and a “simple” quadratic regularizer – \( \lambda \)

De-noise based on advanced prior (\( \beta \))

\[ u = u + (\hat{x} - \hat{v}) \]

Converged

No

Yes

\[ + \]

To plug in prior - design denoising routine using that prior!

4. THE DENOISING PROBLEM

- General inverse problem:
  Estimating $x$ from $y = Ax + w$.

- **Denoising problem** ($A = I; w$: AWGN; GGMRF prior):
  Estimating $x$ from $y = x + w$.

\[
-\log p(y | x) = \frac{1}{2\sigma_w^2} \|y - x\|^2
\]

\[
-\log p(x) = \frac{1}{p\sigma_x^p} \sum_{\{i,j\} \in C} g_{i,j} \left| x_i - x_j \right|^p
\]

- **MAP estimate for $x$:**

\[
\hat{x} = \arg \min_{x \geq 0} \left\{ \frac{1}{2\sigma_w^2} \|y - x\|^2 + \frac{1}{p\sigma_x^p} \sum_{\{i,j\} \in C} g_{i,j} \left| x_i - x_j \right|^p \right\}
\]

$\sigma_w$: Noise Std. Deviation

$\sigma_x$: Regularization parameter

Design parameter, $p = 1.05$
5. NON-LOCAL MEANS (NLM) 

DENOISING

Basic idea:

• NLM filtering takes mean of all pixels in the image, weighted by how similar these pixels (and their neighborhoods) are to the target pixel (and its neighborhood). [1]

Advantage:

• Works great when there are repeating structures. Most images have plenty of similar patches.

Drawbacks:

• Patch match computation is very expensive. 3D implementation of 50x50x50 volume could take about 8 hours to denoise.

• It is not rotationally invariant.

Animation: http://josephsalmon.eu/
NLM IMPLEMENTATION

Implementation:

\[
\hat{x}_i = \frac{\sum_{j \in S} w_{ij} y_j}{\sum_{j \in S} w_{ij}}
\]

NLM Filtering: \( \hat{x}_i \) is the estimate of the pixel \( x_i \) in the noisy image.

Notation:

- \( y_i \): Pixel being denoised.
- \( P_i \): \( N \times N \) neighborhood patch around the pixel ("reference patch")
- \( S \): Set of all pixels.

Reference patch is compared with all other patches, \( P_j \)

Every pixel, \( y_i \), is then weighted as a function of how much its neighborhood \( P_j \) matches with \( P_i \).

Weight computation equation: \( w_{ij} = \exp \left( -\frac{||P_i - P_j||_2^2}{h^2} \right) \)
6. ROTATIONALLY-INVARIANT NON-LOCAL MEANS (RINLM)

Motivation: Regular NLM does not see that the patches in these boxes are exactly the same as the shape outside the boxes.

Our solution: Use rotated versions of the patches to see if they match the patch around the target pixel.
NLM VS. RINLM: AN ILLUSTRATION

Weight assigned in (i) NLM = 4.9997e-04, (ii) RINLM = 1.63e-02.

Weight assigned in RINLM / Weight assigned in NLM = 32.6897
CHALLENGES WITH ROTATION

Two major problems:

• In traditional literature, each patch is rotated \( Q - 1 \) times, where \( Q \) is the total number of pixels in the image.

• For each of those rotation pursuits, every possible angle has to be tried – to see the best match.

Max. total rotational effort in the naïve case: \( 360(Q-1) \) rotations + \( 360(Q-1) \) norm computations!
**SOLUTION: PRE-ROTATION**

**Idea:** Pre-rotate each patch in the image in a pre-specified way.

- Each patch is binarized (to separate foreground from background) and “Center of Mass” (CoM) is computed for each patch.

- The original patch is rotated so that the CoM lies on the negative y-axis. This way all similar shapes are aligned after the pre-rotation step.

\[
CoM_i = \frac{\sum_{i,j} i \cdot y_{ij}}{\sum_{i,j} y_{ij}}; \quad CoM_j = \frac{\sum_{i,j} j \cdot y_{ij}}{\sum_{i,j} y_{ij}}
\]

\(y_{ij}\) is the \((i, j)\)th pixel of the patch to be rotated.

**Advantage:** Each patch has to be rotated only ONCE.
“CENTER OF MASS” ALIGNMENT
PRE-ROTATION ILLUSTRATION

Before pre-rotation

After pre-rotation
7A. RESULTS: PHANTOM

Phantom: super ellipses

Super ellipses model certain structures in materials closely[2].

Size: 256x256 pixels
Type: 8-bit gray-level
Background gray level: 100
Foreground gray level: 200
**Case 1:**

**Low noise level**
(Std. Dev. = 10)

$N$ is the side length of the patch.

- **Noisy image**
  - Std. Dev. = 10
  - RMSE = 4.6764

- **GGMRF (p = 1.05)**
  - RMSE = 3.2880
  - K-SVD
    - RMSE = 3.8096

- **NLM (N = 9, h = 39)**
  - RMSE = 3.9913

- **RINLM (N = 9, h = 39)**
  - RMSE = 3.2880
Case 2: Medium noise level (Std. Dev. = 22.67)

Noisy image
Std. Dev. = 22.67

GGMRF (p = 1.05)
RMSE = 13.0669

K-SVD
RMSE = 7.7943

NLM (N = 5, h = 48)
RMSE = 9.3443

RINLM (N = 5, h = 48)
RMSE = 7.1974
Case 3: High noise level (Std. Dev. = 35)

Noisy image
Std. Dev. = 35

GGMRF (p = 1.05)
RMSE = 21.8152

K-SVD
RMSE = 12.5512

NLM (N = 5, h = 61)
RMSE = 14.2237

RINLM (N = 5, h = 61)
RMSE = 10.2308
7B. RESULTS: PHANTOM WITH SYMMETRIES

Phantom: snowflakes

Snowflakes embody symmetry and fine structure.

Size: 256x256 pixels
Type: 8-bit gray-level
Background gray level: 56
Foreground gray level: 200
Noise
Std. Dev. = 20

Noisy image
Std. Dev. = 20

K-SVD
RMSE = 12.8670

NLM (N = 5, h = 48)
RMSE = 10.1690

RINLM (N = 5, h = 48)
RMSE = 8.6697
7C. RESULTS: NATURAL IMAGE

Image: Cameraman

Size: 256x256 pixels
Type: 8-bit gray-level
Medium noise level (Std. Dev. = 20)

Noisy image
Std. Dev. = 20

GGMRF (p = 1.05)
RMSE = 12.1717

KSVD
RMSE = 9.9874

NLM (N = 9, h = 83)
RMSE = 10.2821

RINLM (N = 9, h = 83)
RMSE = 7.9606
8. CONCLUSION & ON-GOING WORK

- Patch-based methods show a lot of promise when applied as prior models, specially when there are repeating patterns in the image.

- NLM/RINLM are not typically set up as optimization problems. Therefore, we need to employ ADMM-based methods (like the Plug-and-Play framework) to use them for tomography in electron microscopy.

- Ongoing work:
  - Further speed-up techniques for extending RINLM to 3D.
  - Applying RINLM as a prior model (within the Plug-and-Play framework) for tomographic applications.
**FUTURE DIRECTIONS**

- *Cryo-Electron Microscopy to Cryo-Electron Tomography:* Finding a balance between Cryo-EM reconstruction and tomographic reconstruction, use a tilt sequence to reconstruct a single particle → we can make use of additional constraints for better reconstruction as a result of all foreground shapes in a 2D slice resulting from different orientations of one master particle.

- Try to **fuse separate models** for background (like MRF-based) and foreground (dictionary learning based) → this helps achieve dimensionality reduction.
(EXTERNAL) REFERENCES


Thank you!