JOINT ANALYSIS OF X-RAY PTYCHOGRAPHY AND X-RAY FLUORESCENCE

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Inverse Problem Research Group

MULTIMODAL X-RAY DATA

X-Ray Ptychography:

Observations:
- Magnitude/intensities of complex object in Fourier space

Reconstruct:
- Complex object

Goal: Phase retrieval

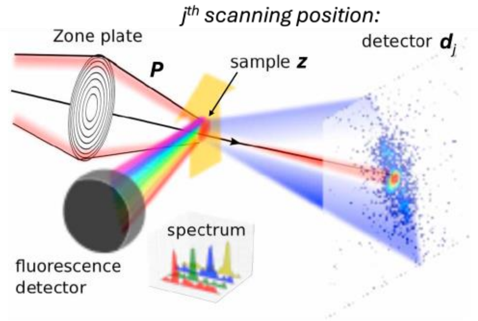


Fig. 1. **Simultaneous ptychographic and fluorescence microscopy.** A focused X-ray beam is scanned across a sample whilst simultaneously recording the X-ray fluorescence spectra and coherent diffraction pattern. [1]

X-Ray Fluorescence:

Observations:
- photons from fluorescent emission

Reconstruct:
- elemental composition and spatial distribution in an object

⇩

"experimental fluorescence map"

Goal: enhance resolution

[1] D. J. Vine et al, Simultaneous X-ray fluorescence and ptychographic microscopy of Cyclotella meneghiniana (2012)

MULTIMODAL APPROACH

⚠️ Individually problems are difficult

Our work:

1. Combine problems in a joint framework
   - ➢ (Hopefully) better-posed
2. Use a commonality between modalities to simplify problem
3. Explore the conditioning of individual and combined problem
4. Run numerical experiments with various setups

X-RAY PTYCHOGRAPHY

$$\boldsymbol{d}_j = \left|\mathcal{F}\left(\boldsymbol{P}_j \boldsymbol{z}\right)\right|^{\mathbf{2}} + \varepsilon_j,$$

- $\boldsymbol{d}_j$ measurements from probe $\boldsymbol{P}$ at $j = 1, \dots, N$ position
- $\boldsymbol{z}$ complex valued object of interest
- $\mathcal{F}$ discrete Fourier

<u>Common optimization methods:</u>

- PIE
  - Steepest descent step for each j
- Multi-grid
  - Better for large-scale problems

$$\min_{\boldsymbol{P},\boldsymbol{z}} \phi^P = \min_{\boldsymbol{P},\boldsymbol{z}} \frac{1}{2} \sum_{j=1}^{N} \left\| \left|\mathcal{F}\left(\boldsymbol{P}_j \boldsymbol{z}\right)\right| - \sqrt{\boldsymbol{d}_j} \right\|_2^2$$

- Non-linear
- Non-convex
  - Depends on overlap of $\boldsymbol{P}_j$

X-RAY PTYCHOGRAPHY

Lack of complex-differentiability ⇒ use Wirtinger calculus

$$\nabla\left(\left|\mathcal{F}\left(\boldsymbol{P}_j \boldsymbol{z}\right)\right| - \sqrt{\boldsymbol{d}_j}\right) = \boldsymbol{J}_j^P = \frac{1}{2}\overline{diag\left(\mathcal{F}\left(\boldsymbol{P}_j \boldsymbol{z}\right)/\left|\mathcal{F}\left(\boldsymbol{P}_j \boldsymbol{z}\right)\right|\right)\mathcal{F}\boldsymbol{P}_j}$$

<u>Gradient of objective function ϕ^P:</u>

$$\nabla\phi^P = \sum_{j=1}^{N} \left(\boldsymbol{J}_j^P\right)^* \left(\left|\mathcal{F}\left(\boldsymbol{P}_j \boldsymbol{z}\right)\right| - \sqrt{\boldsymbol{d}_j}\right)$$

<u>Jacobian:</u>

$$\boldsymbol{J}^P = \begin{bmatrix} \boldsymbol{J}_1^P \\ \vdots \\ \boldsymbol{J}_N^P \end{bmatrix}$$

<u>**Approximate** Hessian:</u>

$$\boldsymbol{H}^P = \left(\boldsymbol{J}^P\right)^T \boldsymbol{J}^P$$

Z. Di, S. Fung (2020), L. Sorber et al, (2012)

X-RAY FLUORESCENCE

$$D_e = |\boldsymbol{P}|^2 * \boldsymbol{w}_e + \hat{\varepsilon}_e$$

- Have experimental fluorescence map D_e of element $e = 1, \dots, N_e$
- Can use $\boldsymbol{P}$ from ptychography to enhance resolution

$$\min_{\boldsymbol{P},\boldsymbol{w}_e} \phi^F = \min_{\boldsymbol{P},\boldsymbol{w}_e} \sum_{e=1}^{N_e} \left|\left| \, |\boldsymbol{P}|^2 * \boldsymbol{w}_e - D_e \, \right|\right|_2^2$$

- Blind-deconvolution

Current approach:

1. Solve blind ptychography and obtain probe $\boldsymbol{P}$
2. Use $\boldsymbol{P}$ to deconvolve D_e

D. J. Vine et al, Simultaneous X-ray fluorescence and ptychographic microscopy of Cyclotella meneghiniana (2012)

X-RAY FLUORESCENCE

First note:

$$|\boldsymbol{P}|^2 * \boldsymbol{w}_e = \widehat{\boldsymbol{P}}\boldsymbol{w}_e$$

- $\widehat{\boldsymbol{P}}$ is the matrix representation of the 'same' convolution (preserves dimension)

Gradient of objective function ϕ^F:

$$\nabla\phi^F = \sum_{e=1}^{N_e} \widehat{\boldsymbol{P}}^T(\widehat{\boldsymbol{P}}\boldsymbol{w}_e - D_e)$$

Jacobian:

$$\boldsymbol{J}_e^F = \widehat{\boldsymbol{P}}, \qquad \boldsymbol{J}^F = \begin{bmatrix} \widehat{\boldsymbol{P}} \\ \vdots \\ \widehat{\boldsymbol{P}} \end{bmatrix} \} N_e\ times$$

Hessian:

$$\boldsymbol{H}^F = (\boldsymbol{J}^F)^T \boldsymbol{J}^F$$

JOINT FRAMEWORK

Introduce joint objective for a better-posed problem

$$\min_{\boldsymbol{w},\boldsymbol{P},\boldsymbol{z}} \alpha \sum_{e=1}^{N_e} \left\| \, |\boldsymbol{P}|^2 * \boldsymbol{w}_e - D_e \, \right\|_2^2 + \frac{1}{2} \sum_{j=1}^{N} \left\| \, \left|\mathcal{F}\left(\boldsymbol{P}_j \boldsymbol{z}\right)\right| - \sqrt{\boldsymbol{d}}_j \right\|_2^2$$

- α balances the two objectives

Commonality between modalities:

$$\boldsymbol{z} = \boldsymbol{\delta} + i\boldsymbol{\beta}, \qquad \boldsymbol{\delta} = \sum_e \boldsymbol{w}_e \mu_e \qquad \text{(assume } \mu_e = 1\text{)}$$

$$\phi = \min_{\boldsymbol{w},\boldsymbol{P},\boldsymbol{\beta}} \alpha \sum_{e=1}^{N_e} \left\| |\boldsymbol{P}|^2 * \boldsymbol{w}_e - D_e \, \right\|_2^2 + \frac{1}{2} \sum_{j=1}^{N} \left\| \left|\mathcal{F}\left(\boldsymbol{P}_j \left(\Sigma_e \boldsymbol{w}_e + i\boldsymbol{\beta}\right)\right)\right| - \sqrt{\boldsymbol{d}}_j \right\|_2^2$$

JOINT APPROACH

Gradient of objective function ϕ:

$$\nabla\phi = \alpha\nabla\phi^F + \nabla\phi = \alpha\sum_{e=1}^{N_e}\widehat{\boldsymbol{P}}^T\left(\widehat{\boldsymbol{P}}\boldsymbol{w}_e - D_e\right) + \sum_{j=1}^{N}\left(\boldsymbol{J}_j^P\right)^*\left(\left|\mathcal{F}\left(\boldsymbol{P}_j\boldsymbol{z}\right)\right| - \sqrt{\boldsymbol{d}}_j\right)$$

Jacobian:

$$\boldsymbol{J} = \begin{bmatrix}\alpha\boldsymbol{J}^F \\ \boldsymbol{J}^P\end{bmatrix}$$

Approximate Hessian:

$$\boldsymbol{H} = \alpha(\boldsymbol{J}^F)^T\boldsymbol{J}^F + (\boldsymbol{J}^P)^T\boldsymbol{J}^P$$

Question: Is the joint system better conditioned?

NUMERICAL EXPERIMENTS

- To simplify problem
  - fix probe at ground truth
  - Set $N_e = 1$
- Truncated newton (TN) optimization solver
  - Hessian-free
  - Uses finite difference of Jacobians to approximate $\boldsymbol{H}$
- Vary probe overlap, problem size, and element channel

Two Experiment Setups:

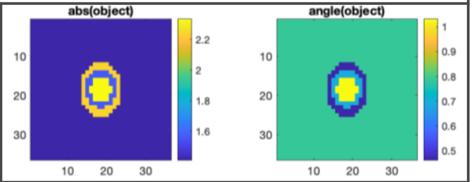
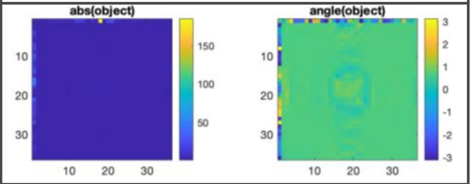
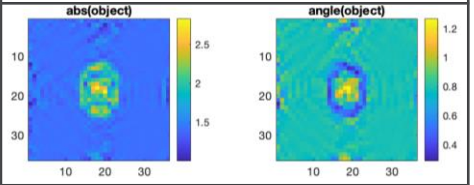
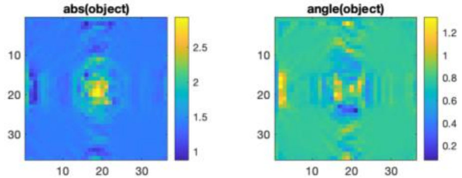
1. Alternate between TN for ptychography ϕ^P and TN for fluorescence ϕ^F
2. Use TN for full joint problem ϕ

RESULTS: SMALL EXAMPLE

Experimental Setup:

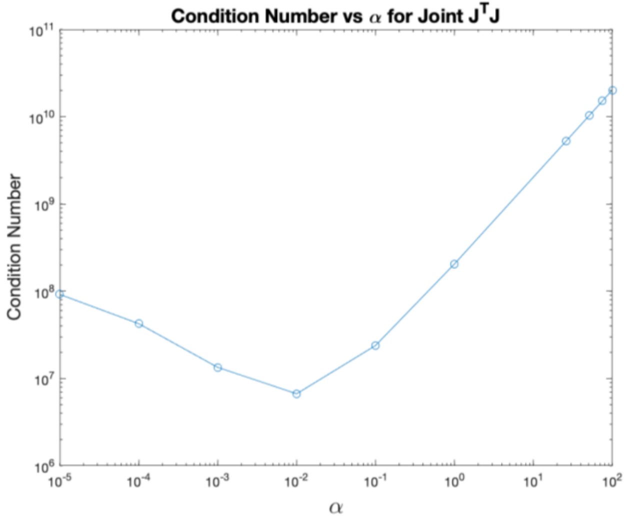
- Probe:
- 9 scanning locations
- Overlap:

- 600 objective function eval

Magnitude and Phase Recon. (fixed probe)	
True	
Ptychography Only	
Joint Framework	
Alternating Framework	

HESSIAN ANALYSIS: SMALL EXAMPLE

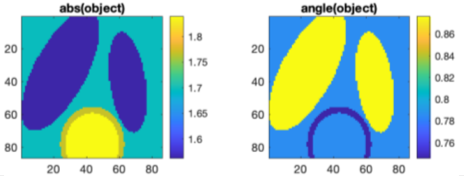
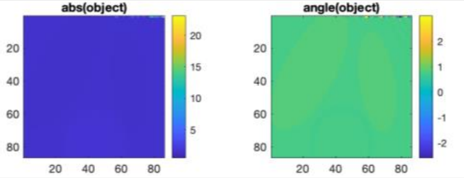
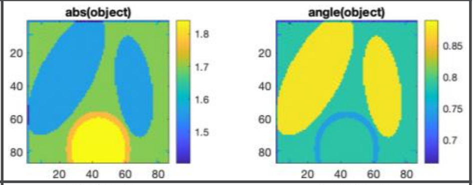
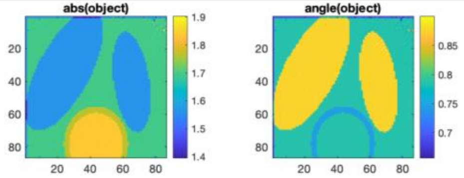
Analysis of $J^T J$	
	Cond. Num.
Ptychography	8.80e+11
Fluorescence	3.75e+19
Combined	6.68e+06



RESULTS

<u>Experimental Setup:</u>
- Probe: 36x36
- 36 scanning locations
- Overlap: 72%

- 600 objective function eval

Magnitude and Phase Recon. (fixed probe)	
True	
Ptychography Only	
Joint Framework	
Alternating Framework	

RESULTS:

Experimental Setup:

- Probe: 64x64
- 36 scanning locations
- Overlap: 84%

- 600 objective function eval

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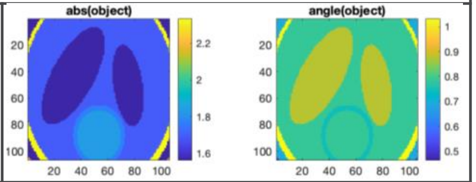
<tr><td>True</td><td>
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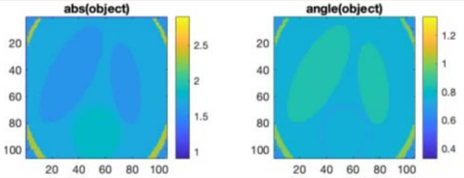
<tr><td>Ptychography Only</td><td>
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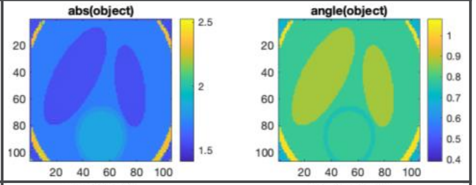
<tr><td>Joint Framework</td><td>
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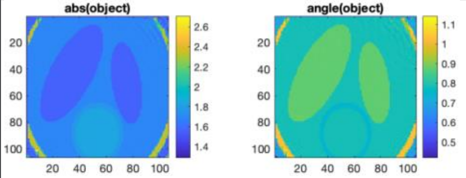
<tr><td>Alternating Framework</td><td>
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CONCLUSIONS

- Combining modalities can improve the conditioning of the system
- Joint approach may lead to better reconstructions

Future Directions:

- Numerical tests on various experimental configurations
  - Problem size
  - Scanning overlap
  - Noise level
- Rigorous quantification of multimodal benefit

THANK YOU!!! QUESTIONS?