Ptychographic Inversion and Uncertainty Quantification using Invertible Neural Networks

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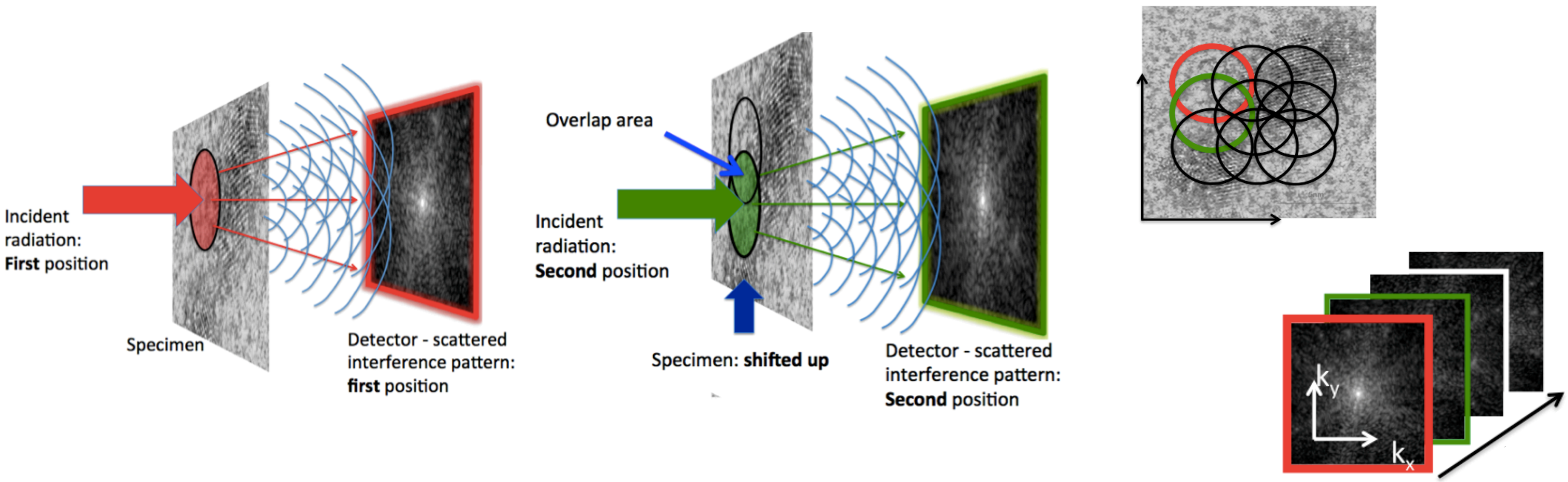
Ptychography



Lensless, scanning,

coherent diffraction imaging technique

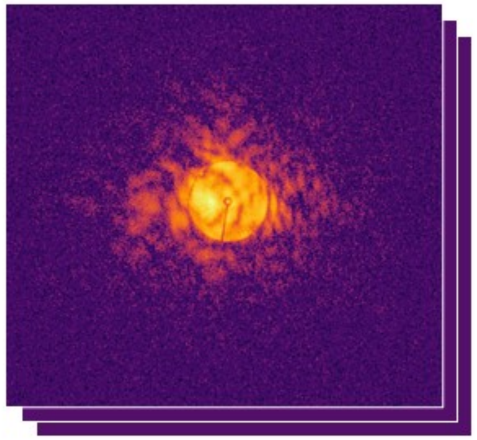
Rodenburg, John M. "Ptychography and related diffractive imaging methods." *Advances in Imaging and Electron Physics* 150 (2008): 87-184.

Inverse problem

Complex object: $\mathbf{z} = \mathbf{x} + i\mathbf{y} \in \mathbb{C}^{n\times n}$

Data — diffraction patterns: $\mathbf{d} = f(\mathbf{z}) + \epsilon$

$$d_j = |\mathcal{F}(\mathbf{P}_j\mathbf{z})|^2 + \epsilon_j, \quad j = 1,\ldots,N$$



Scanning overlapping regions makes inversion possible

Traditional approach:

point estimates,

no indication of solution quality

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

Challenges:

High dimensionality, non-convex, nonlinear forward model

Bayesian Inversion

Account for all possible solutions through the posterior distribution :

$$\pi(\mathbf{z} \mid \mathbf{d})$$

Non-convexity → *Multimodal posterior*

Nonlinear → *Non-Gaussian*

High dimensional → *Difficult to apply MCMC*

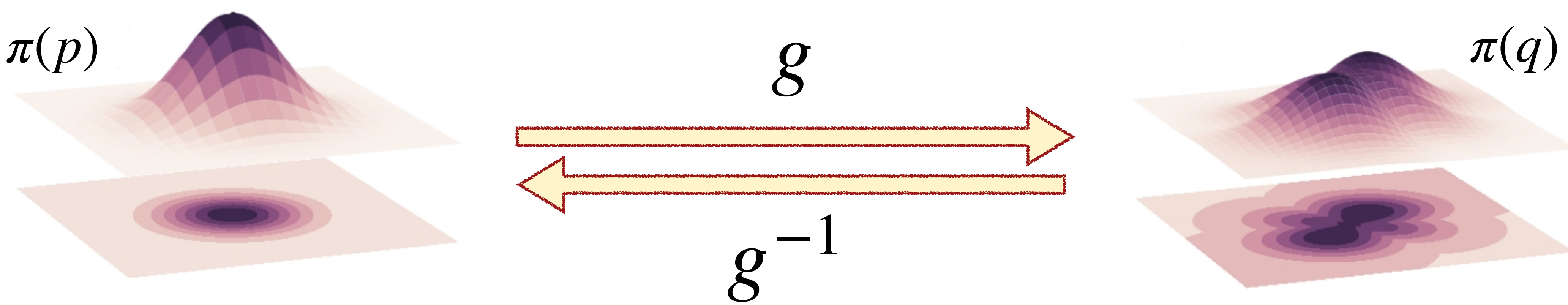
Variational inference

$$\pi(\mathbf{z} \mid \mathbf{d}) \approx \pi(\mathbf{z}; \mathbf{d}, \theta)$$

Need an expressive model to capture the complicated posterior

Use **normalizing flows** to approximate the posterior

Normalizing flows



simple *distribution*

$$\pi(p) = \pi(q) \left| \det \nabla_q g(p;\theta) \right|^{-1}$$

complex target *distribution*

Ingredients

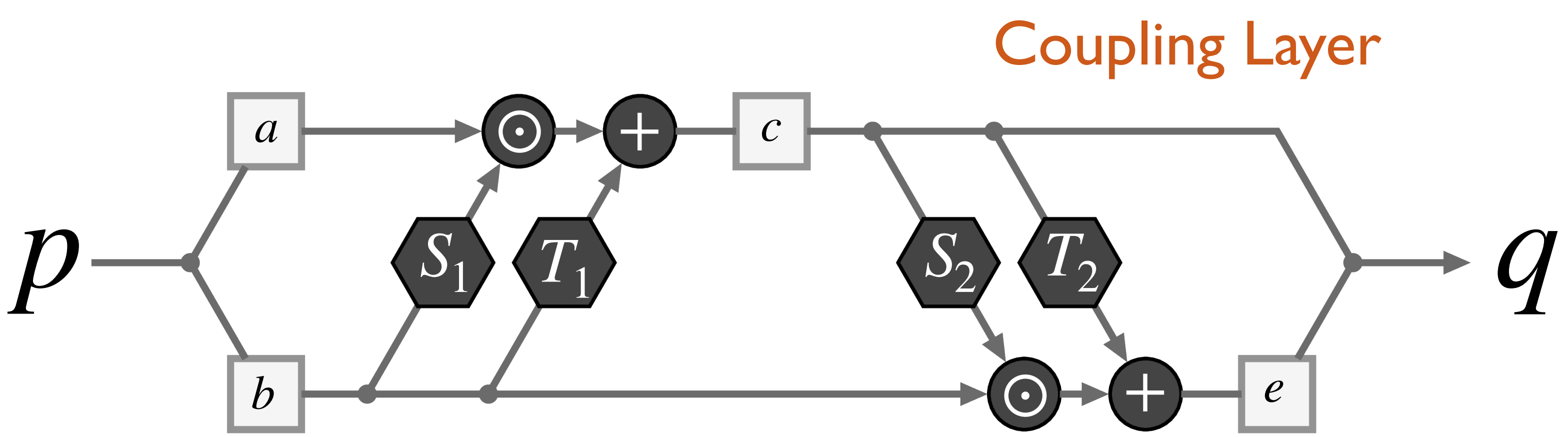
1. A simple distribution
2. An invertible map
3. Change of variables

Features

1. Exact likelihood computations
2. Tractable Jacobian computations
3. Expressive

Kobyzev, Ivan, Simon JD Prince, and Marcus A. Brubaker. "Normalizing flows: An introduction and review of current methods." *IEEE Transactions on Pattern Analysis and Machine Intelligence* 43.11 (2020): 3964-3979.

Invertible neural networks



$$p = \begin{bmatrix} a \\ b \end{bmatrix} \qquad \begin{aligned} c &= a \odot S_1(b) + T_1(b) \\ e &= b \odot S_2(c) + T_2(c) \end{aligned} \qquad \begin{bmatrix} c \\ e \end{bmatrix} = q$$

Easier to compute Jacobians

Flow = Activation normalization + permutation + coupling layer

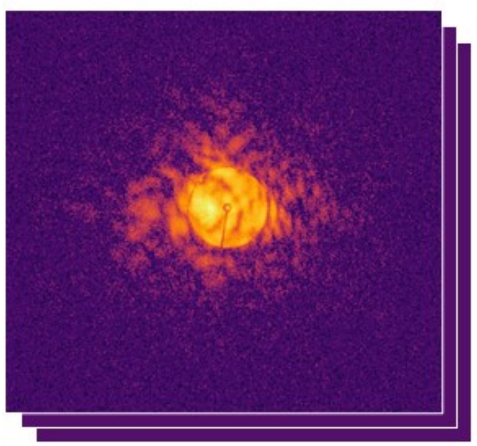
Dinh, L., Sohl-Dickstein, J., & Bengio, S. (2016). *arXiv preprint arXiv:1605.08803*.

Proposed approach

Likelihood model

$$\mathbf{d} = f(\mathbf{z}) + \epsilon$$

Data



Variational inference

Invertible Neural Network → **Posterior Distribution**

Loss function

$$\theta^* = \operatorname{argmin}_\theta \sum_{j=1}^{B} l(\mathbf{d}, f(g(\mathbf{z}^{(\mathbf{j})};\theta))) + \lambda \mathscr{R}(\mathbf{g}(\mathbf{z}^{(\mathbf{j})};\theta)) - \log \left| \det \frac{\partial \mathbf{g}(\mathbf{z}^{(\mathbf{j})};\theta)}{\partial \mathbf{z}^{(\mathbf{j})}} \right|$$

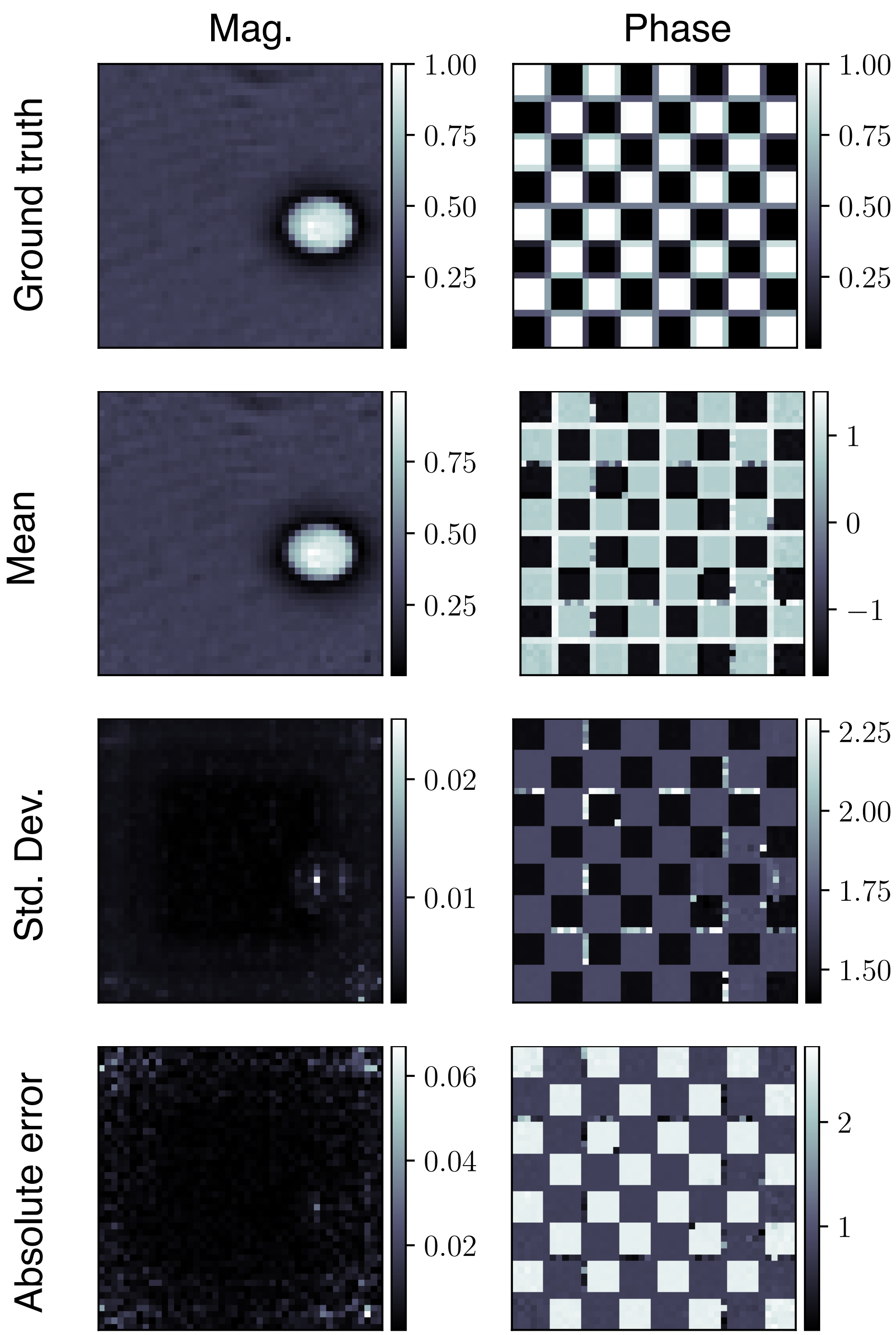
Data misfit **Regularization** **Implicit regularization**

Sun, H., & Bouman, K. L. (2020). *arXiv preprint arXiv:2010.14462, 9*.

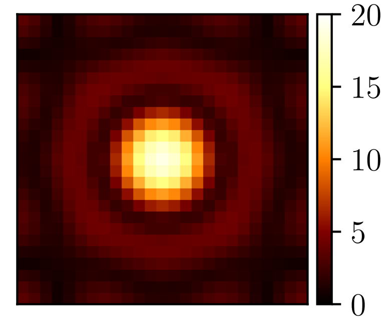
Ardizzone, L., et. al. (2018). *arXiv preprint arXiv:1808.04730*.

Results

Synthetic object

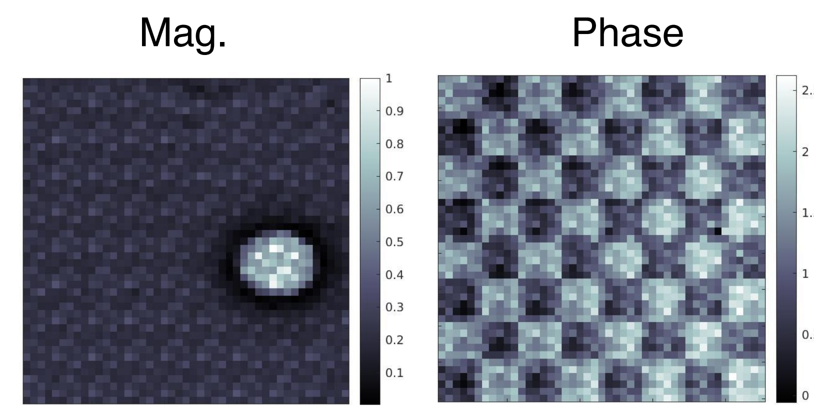


Probe

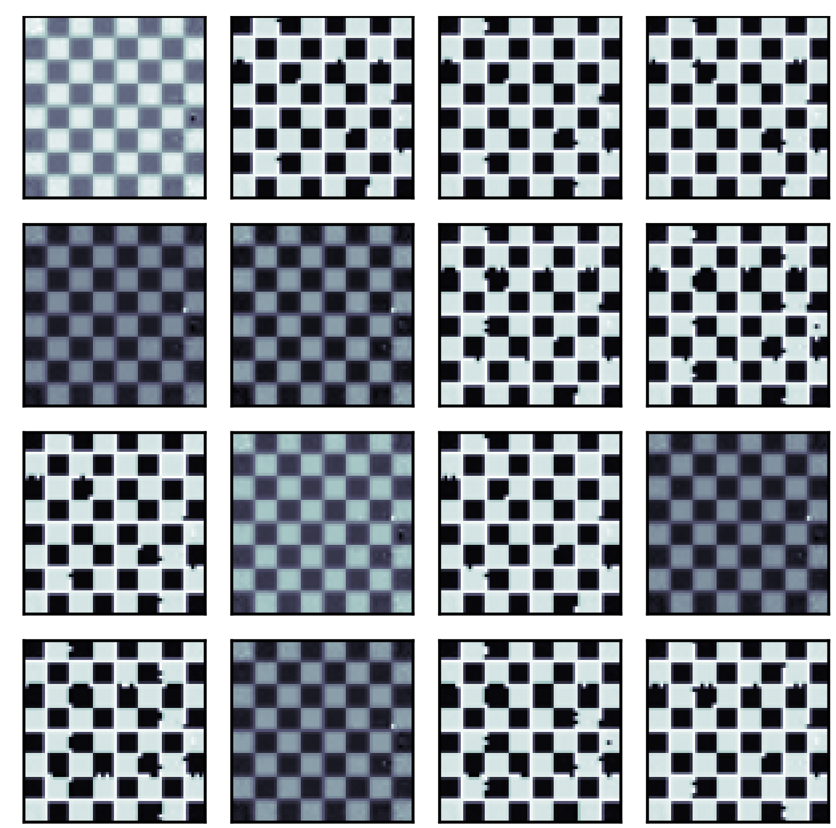


Object is scanned 25 times
Overlap ratio : 0.8
1% noise in measurements

Reconstruction from rPIE

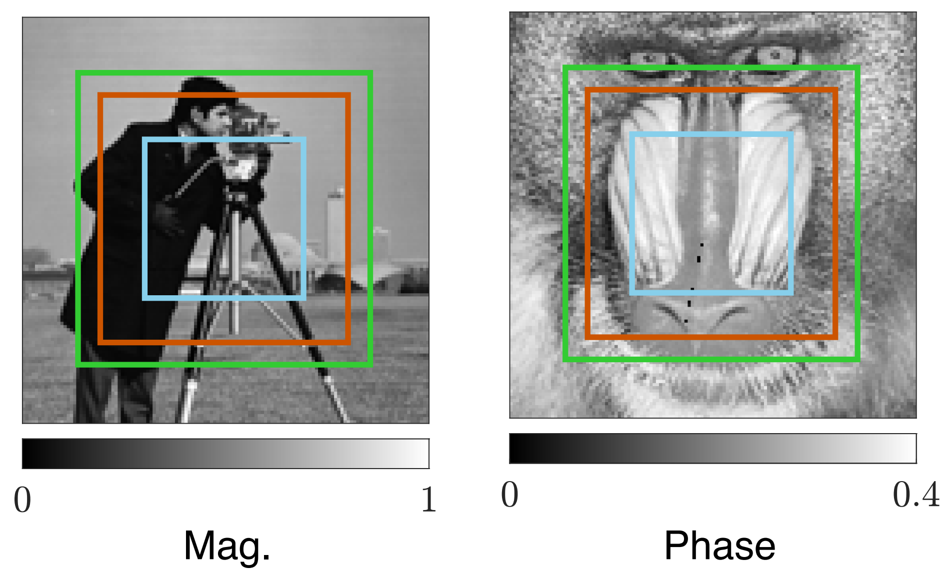


Multi-modal posterior

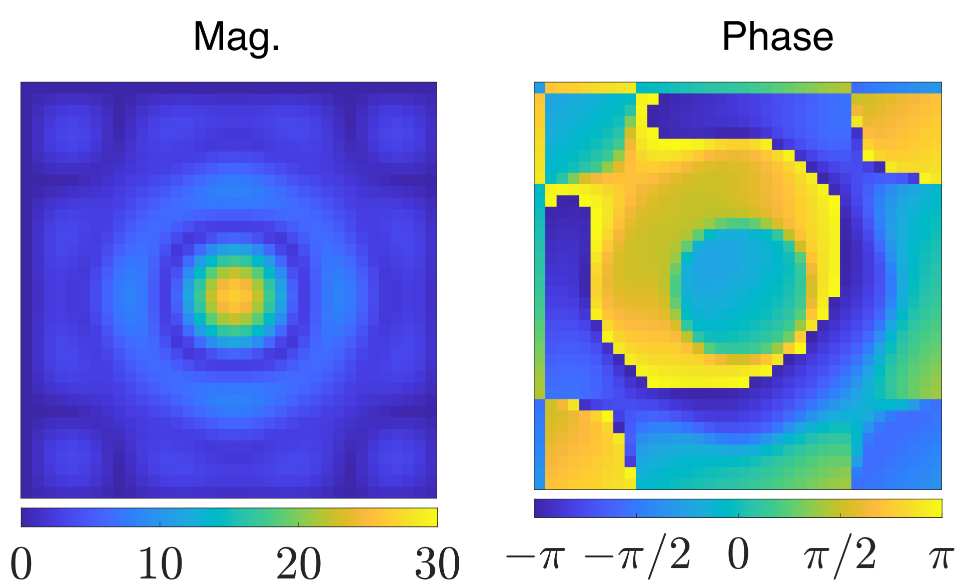


Results

Synthetic object



Complex Probe



Numerical study:

1. Probe is of size 36 X 36

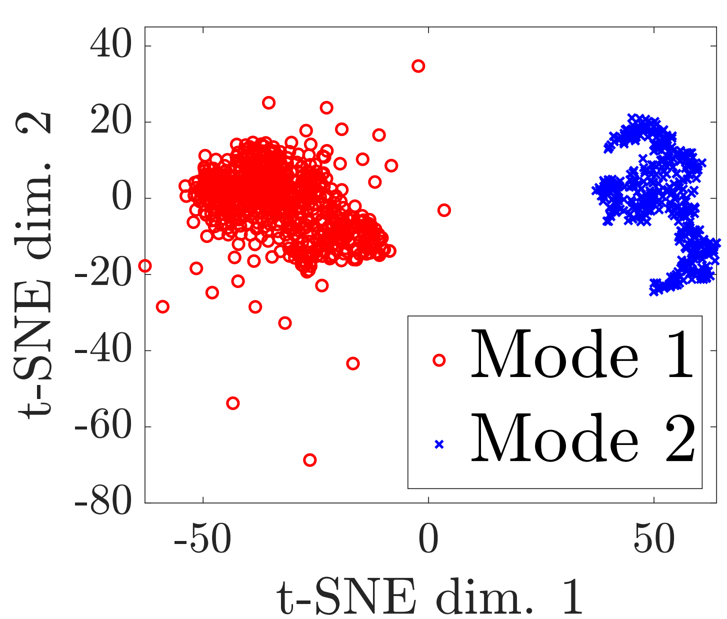
2 .Object is scanned 64 times

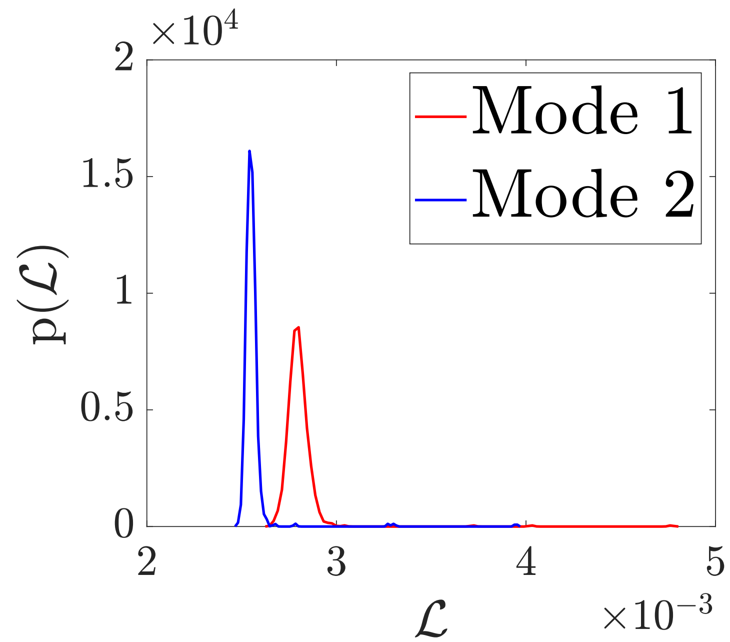
3. 64 X 36 X 36 measurements

4. 3 settings with different FOV

5. 1% noise in measurements

Results

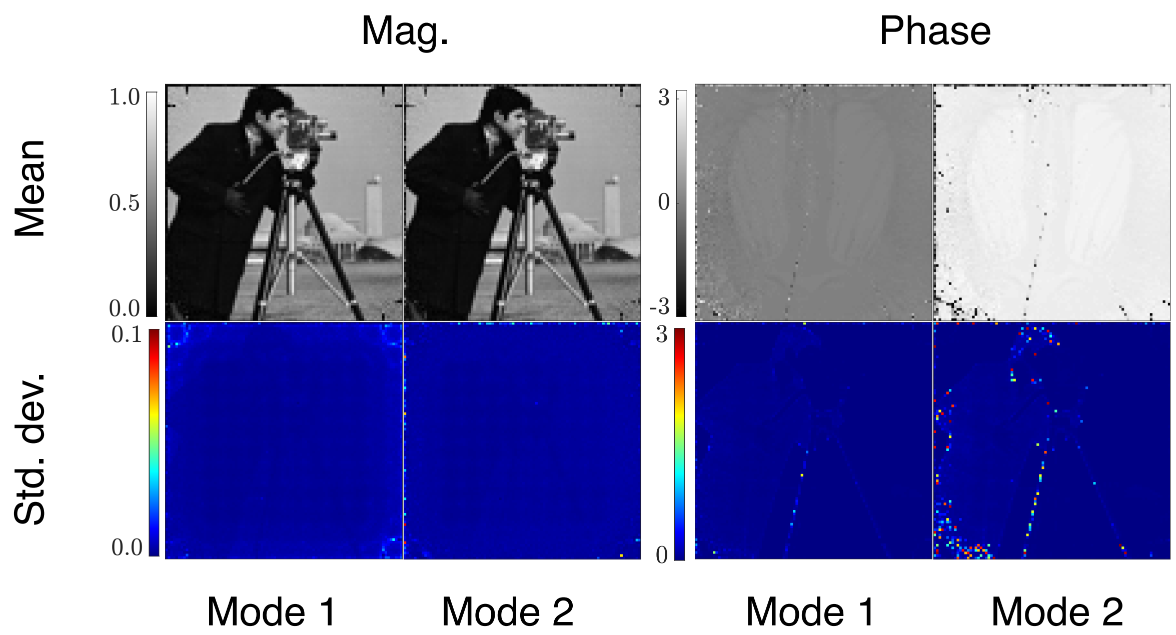


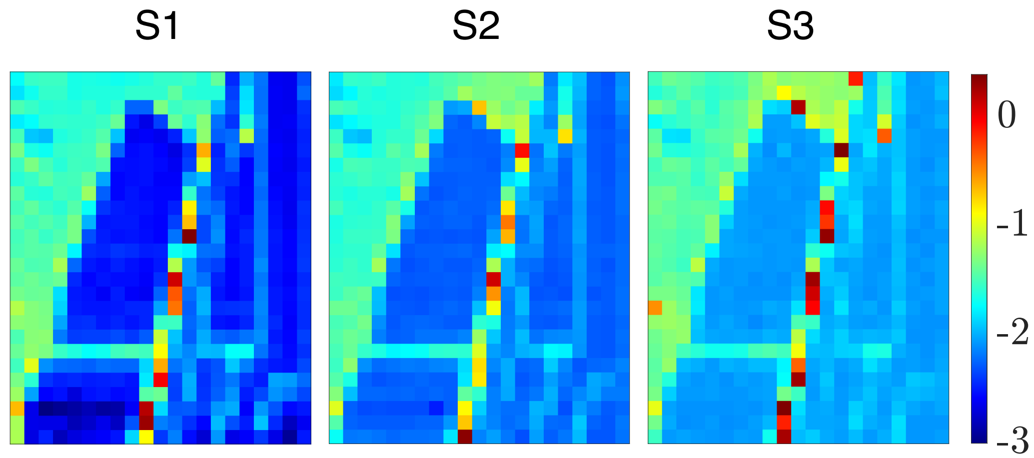


Multimodal posterior

We observed that the NF model was able to capture **two modes** of the posterior

Results





Increasing overlap reduces uncertainty

Scan Setting	FOV n	Overlap Ratio	Recon. Mag. PSNR / Recon. Phase SSIM		
			NF Mode 1	NF Mode 2	rPIE
$S1$	50	0.94	26.69/0.48	26.64/0.54	26.82/0.25
$S2$	78	0.83	22.77/0.20	23.66/0.39	23.08/0.18
$S3$	92	0.78	21.20/0.50	22.69/0.44	22.32/0.16

Good reconstructions compared to rPIE

+

Uncertainty Quantification

Conclusions and outlook

Summary:

1. Normalizing flows enable ptychographic inversion via variational inference.
2. Good reconstruction with uncertainty quantification
3. Multimodal solution characterization

Future directions:

1. Interpret the modes of the posterior
2. Scalability to larger problems
3. Exploiting partial data for local solution

Paper

Acknowledgements

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