

Research Proposal: Partially coherent ptychography

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1 Introduction and objectives

Ptychography is a popular imaging technique in scientific fields as diverse as condensed matter physics, cell biology, materials science, and electronics, among others. In a coherent Ptychography experiment, a localized coherent X-ray probe (or illumination) scans through a specimen, while the detector collects a sequence of phaseless intensities in the far-field. The goal is to obtain a high-resolution reconstruction of the specimen from the sequence of intensity measurements.

Coherent Ptychographic imaging experiments often rely on apertures to define a coherent illumination. Research institutions around the world are investing considerable resources to produce brighter x-ray sources to overcome this limitation. Meanwhile, most of the x-ray photons generated are currently discarded by secondary apertures. Even when there is enough coherent flux, the stability required during exposure is often another limiting factor. In a word, coherent light sources need strict experiment conditions and could cause waste. Both flux and stability limitations can be reduced using partial coherence analysis.

To characterize a partially coherent effect, different forward models are proposed. A general model is proposed by physicists in [3], which is a blind ptychography model based on quantum state tomography. Phobe is assumed to be in a mixed state with r modes. Algorithms like Alternative projection(AP) could be extended from the coherent case to find the r main components. In another view, we are reconstructing an approximated rank- r density matrix. Although

this model reconstructed images successfully in various cases like fly-scan data with translational blur, the physical interpretation of the multiple modes is unclear, and the relationship with the coherence function is indirect. Therefore, some specific models are proposed for different experimental settings[9].

In [1] the authors characterize the partially coherent effect as a blur on the main probe ω with vibration kernel κ . Because this forward model is hard to compute, they used Gradient Decomposition of the Probe (GDP), a new forward model to approximate it. Then they presented GDP-ADMM, an iterative solver that jointly optimizes the image, the probe, and the variance of the kernel function. However, when the size of the kernel increases, the approximation accuracy drops, and the results seem blurry. And they assumed the kernels to be gaussians and optimize the variance parameters only, which may not fit the real-world data. In another simpler model, the partially coherent effect is characterized by adding a blur to the measurements in a coherent case. It can be interpreted as blurring or binning multiple pixels at the detector.

In this paper, we would like to characterize partially coherent in the mathematical language and design an effective algorithm to solve the problem. We would mainly focus on the vibration model in [1], combine the advantages of different models, and get a model with both good generalization ability and interpretation ability. And then, we would design an algorithm utilizing the special structure of the model, and conduct numerical experiments to show its efficiency. To theoretically prove the rationale of the model and algorithm, quantitative analysis is required to characterize the approximation error of the model and the convergence speed of the algorithm, under suitable assumptions for the probe ω and the vibration kernel κ .

2 Methods

To combine models used in different settings, we would like to build connections between them through applied analysis skills and prove the equivalency under suitable assumptions. To obtain a high-resolution reconstruction of the specimen from the sequence of intensity measurements, we need to solve an inverse problem, which would be described as an optimization problem.

There are plenty of optimization algorithms available, like the Gradient descent method. Considering the non-convex and low-rank nature of this problem, we would try algorithms in these fields [11][12]. In the vibration model, the low-rank density matrix is generated by the main mode ω instead of a general one, so we hope to make innovative adjustments utilizing the structure inside.

The algorithm would first be tested on simulation data. Then, we would get data from SLAC National Accelerator Laboratory and test on real-world data. For non-convex optimization, we could follow the general framework in [10] to conduct convergence analysis as did in [8].

3 Background/prior work

1. Model

The general model in [3]:

$$\begin{aligned} &\text{Find } u, r \text{ outhogonal } w_k \text{ s.t.} \\ f_{pc,j} &= \sum_{k=1}^r |\mathcal{F}(\mathcal{S}_j u \circ (\omega_k))|^2 \quad (0 \leq j \leq N-1) \end{aligned} \quad (3.1)$$

Another form of 3.1:

$$\begin{aligned} &\text{Find } u, \rho, \text{ s.t.} \\ f_{pc,j}(q) &= \text{Tr}(\mathcal{I}_{j\mathbf{q}}\rho) \quad (0 \leq j \leq N-1) \\ &\rho \text{ is positive semi-definite, with rank } \leq r \end{aligned} \quad (3.2)$$

[9] and the vibration model [1] are two specific ones:

$$f_{pc} = f * \kappa \quad (3.3)$$

$$f_{pc,j} = \sum_i \kappa_i |\mathcal{F}(\mathcal{S}_j u \circ (\mathcal{T}_i \omega))|^2 \quad (3.4)$$

We have shown that model 3.4 is a special case of model 3.1 that approximates a partially coherent effect with a low-rank matrix. Our numerical experiment shows that the density matrix ρ in the vibration model is approximated low-rank, which is consistent with previous literature though the suitable number of states r remains empirical.

Based on the equivalency above, we could generate an ideal density matrix for a vibration kernel κ , use SVD to decompose it, and get the standard mode pattern. Symmetrical and beautiful modes appeared like in [1], some of which are similar to derivations (especially the first and the second orders) of the main mode ω . We used Functional expansion skills like Taylor expansion to expand the probe under smooth conditions and got primary explanations. Investigating the origin of the mode pattern helps understand the structure inside the low-rank matrix and provide insights for an innovative algorithm design.

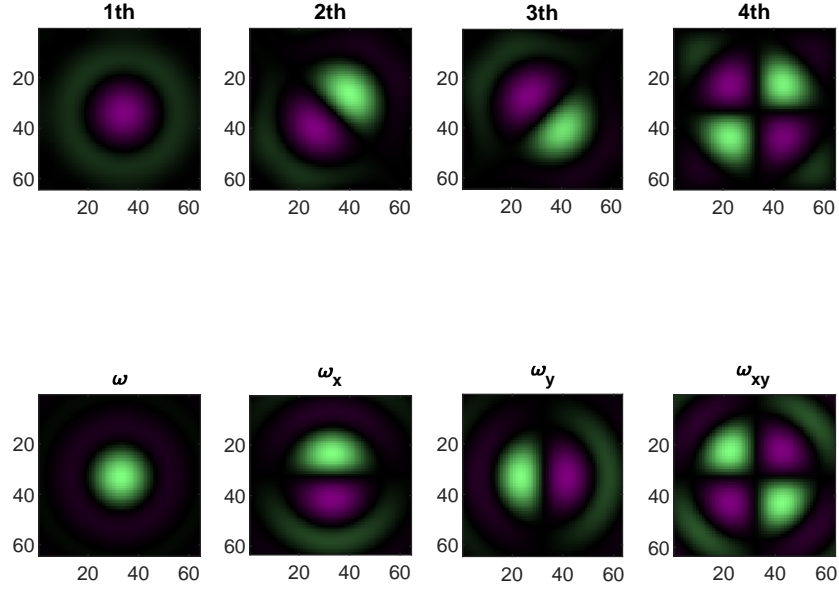


Figure 1: Decomposed modes

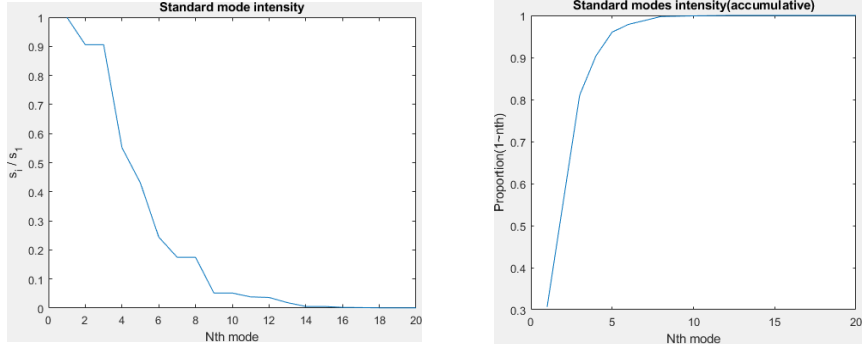


Figure 2: The distribution of singular values of the standard density matrix ρ . The vertical axis in the left subfigure represents the ratio of i^{th} largest singular to the first one s_i/s_1 , and that in the right one represents $S_{cum}(i)$. The singular value decreases exponentially and the matrix is approximately low-rank.

2. Problem solving

ADMM algorithm has been used to solve coherent Ptychography problem with convergence analysis[8]. In a partially coherent problem, an intuitive AP(alternative projection) algorithm was commonly used. We firstly extended the ADMM algorithm to mixed states, and then tried adjustments to supplement the searching process, like adding orthogonal constraints.

We conducted simulation experiments similar to [1] and introduced performance metrics like R-factor and SNR to evaluate the reconstructed results

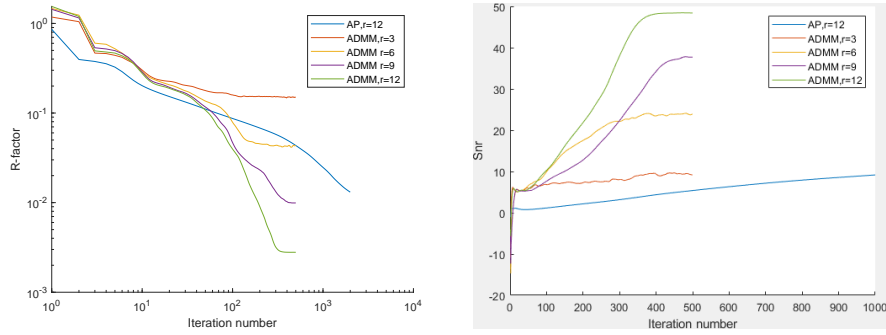
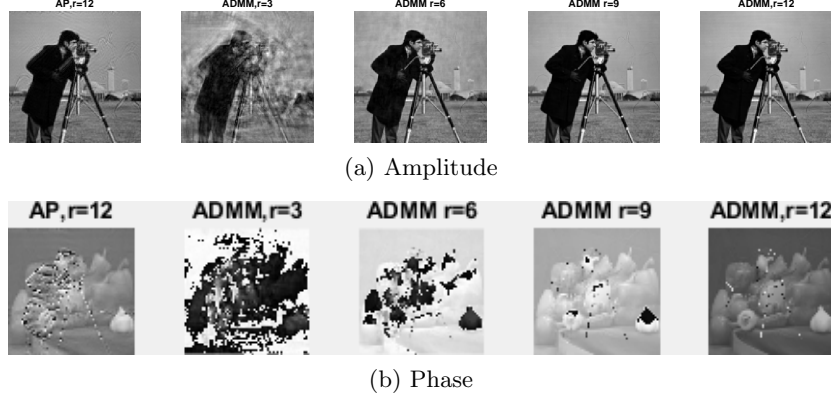


Figure 4: R and snr.

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