Research Proposal: Partially coherent ptychography

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1 Introduction

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.

2 Objectives

Generally speaking, we would like to characterize partially coherent to Mathematical language and design an effective algorithm to solve the problem. To 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 phobe and the vibration kernel for a partially coherent effect.

3 Methods

1. Model

   Models would be borrowed from physics literature and transformed into mathematical language. Because various models are used to characterize partially coherent effects in different settings, we would like to build connections between models through applied analysis skills. 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.

2. Algorithm

   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 focus on algorithms in these fields [11][12], and make innovative adjustments utilizing the structure inside the specific model.

3. Experiment

   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.

4. Convergence Analysis

   For non-convex optimization, we could follow the general framework in [10].

4 Background/prior work

1. Model

   We would mainly investigate three models. [3] proposes a general model based on quantum state tomography. The phobe is assumed to be in a mixed state to represent a partially coherent effect.

$$\begin{aligned} &\text{Find } u, r \text{ othogonal } w_k \ s.t. \\ &f_{pc,j} = \sum_{k=1}^{r} \left| \mathcal{F}\left(\mathcal{S}_j u \circ (\omega_k)\right)\right|^2 (0 \leq j \leq N-1) \end{aligned} \tag{4.1}$$

Another form:

$$\begin{aligned}
&\text{Find } u, \rho, s.t. \\
&f_{pc,j}(q) = Tr(\mathcal{I}_{j\mathbf{q}}\rho)(0 \le j \le N-1) \\
&\rho \text{ is positive semi-definite, with rank} \le r
\end{aligned} \tag{4.2}$$

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

$$f_{pc} = f * \kappa \tag{4.3}$$

$$f_{pc,j} = \sum_i \kappa_i \left|\mathcal{F}\left(\mathcal{S}_j u \circ (\mathcal{T}_i \omega)\right)\right|^2 \tag{4.4}$$

We have shown that 4.4 in a special case of 4.1. Though numerical experiment shows that the density matrix ρ in vibration model is approximated low-rank, no theoretical analysis has been conducted, and the suitable number of states remains empirical. Besides, the decomposed modes are amazingly beautiful, some of which are similar to derivations of the main mode. We used Functional expansion skills like Taylor expansion to expand the phobe under some smooth conditions and got primary explanations.

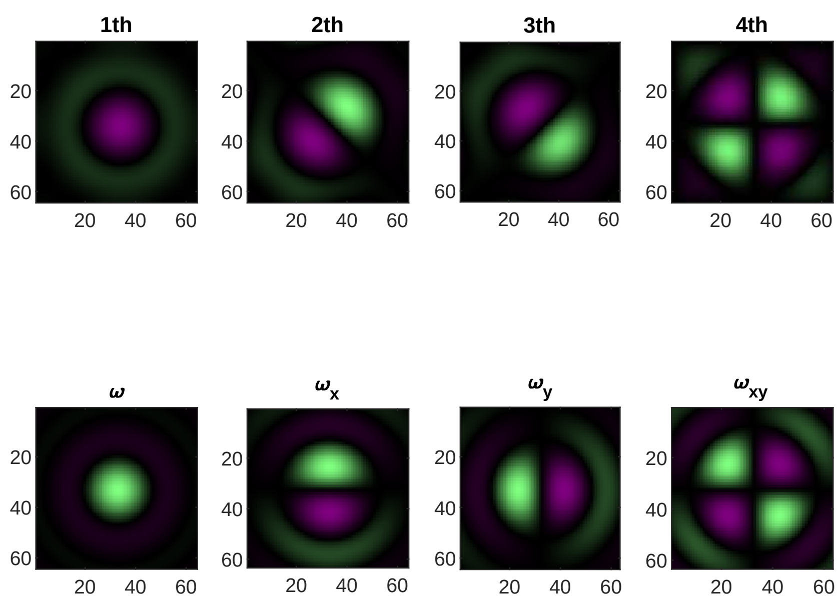


Figure 1: Decomposed modes

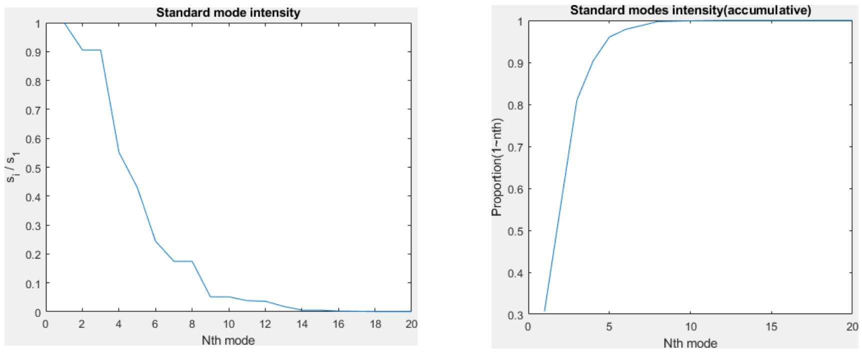


Figure 2: The distribution of singular values of the standard density matrix ρ. The vertical axis in the left subfigure represents the ratio of i^{th} largest singular to the first one s_i/s_1, and that in the right one represents $S_{cum}(i)$. The singular value decreases exponentially and the matrix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

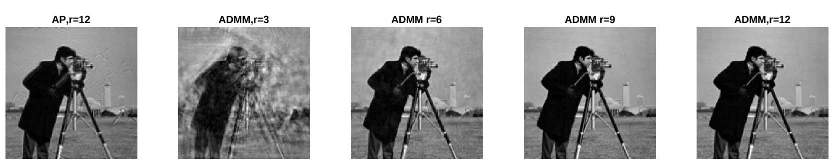
2. Problem solving

   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.

3. Experiment

   We used a general model and extended ADMM algorithm, conducting Experiments similar to [1]. Our methods could overcome larger partially coherent effects, and experiment results show greater speed over AP.

Figure 3



(a) Amplitude

(b) Phase

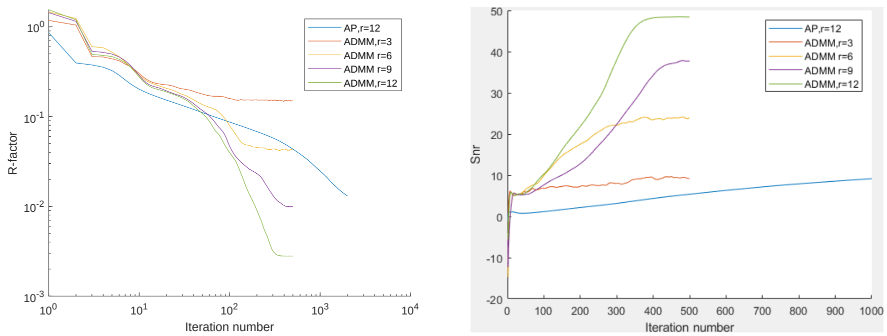


Figure 4: R and snr.

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