

# 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 probe 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 probe is assumed to be in a mixed state to represent a partially coherent effect.

Find  $u, r$  orthogonal  $w_k$  s.t.

$$f_{pc,j} = \sum_{k=1}^r |\mathcal{F}(\mathcal{S}_j u \circ (\omega_k))|^2 \quad (0 \leq j \leq N-1) \quad (4.1)$$

Another form:

Find  $u, \rho$ , s.t.

$$f_{pc,j}(q) = \text{Tr}(\mathcal{I}_{j\mathbf{q}}\rho) (0 \leq j \leq N-1) \quad (4.2)$$

$\rho$  is positive semi-definite, with  $\text{rank} \leq r$

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

$$f_{pc} = f * \kappa \quad (4.3)$$

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

We have shown that 4.4 is a special case of 4.1. Though numerical experiment shows that the density matrix  $\rho$  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 probe under some smooth conditions and got primary explanations.

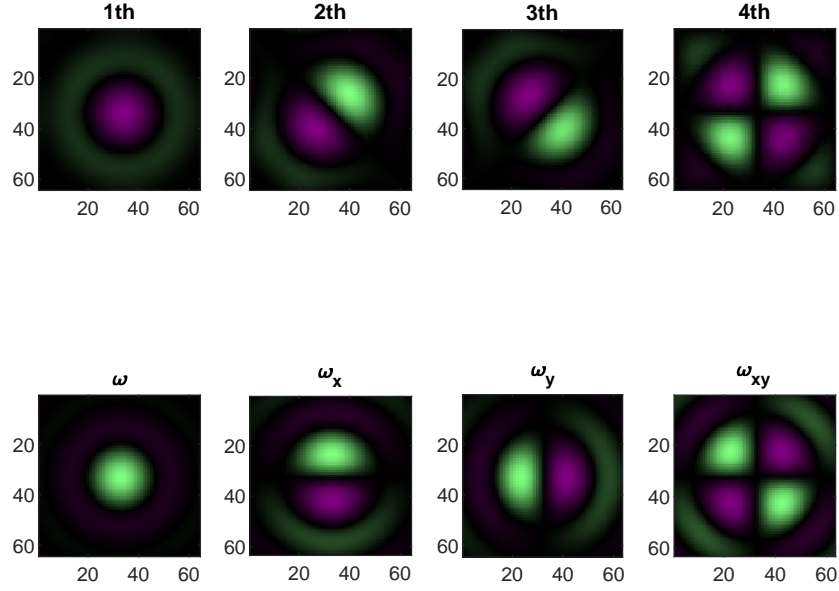


Figure 1: Decomposed modes

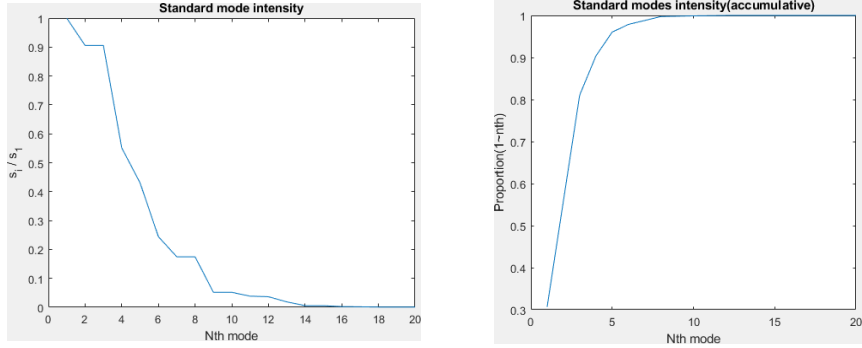


Figure 2: The distribution of singular values of the standard density matrix  $\rho$ . The vertical axis in the left subfigure represents the ratio of  $i^{th}$  largest singular to the first one  $s_i/s_1$ , and that in the right one represents  $S_{cum}(i)$ . The singular value decreases exponentially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

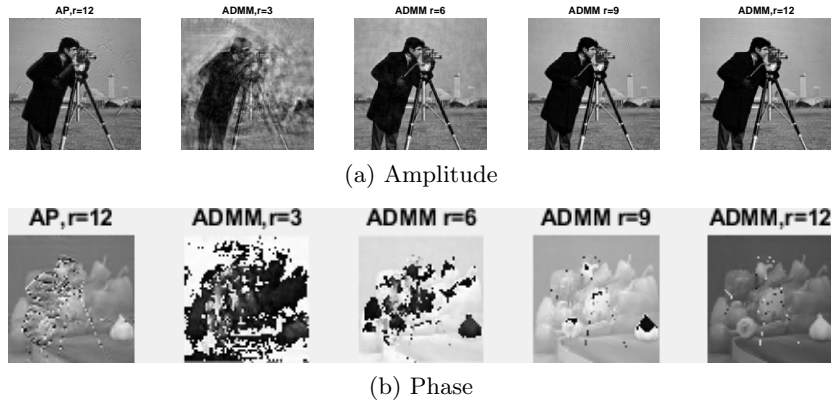
## 2. Problem solving

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



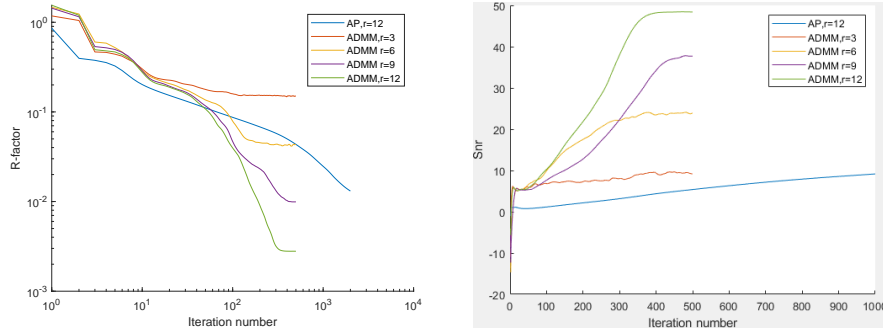


Figure 4: R and snr.

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Tong has a convincing reason of her research interest – computational and applied mathematics, especially in digital signal and image processing, and their applications in medicine and neuroscience. First, it is what she is good at and loves. She learned to implement data structures and algorithms in C++ from the first grade of junior high school and got a solid computing foundation through six years of training in programming and algorithm. She participated in the National Youth Computer Competition on behalf of her senior middle school and won the first prize of the National Olympiad in Informatics in Provinces. She showed even stronger interest in Mathematics - in her words, she is obsessed with the abstraction and simplicity of mathematical language.

Moreover, the predicament encountered by her family gave her an extraordinary enthusiasm and interest in solving medical problems with mathematical tools. We are sorry to know that she lost her father because of brainstem hemorrhage, and her mother-in law was admitted to the hospital because of schizophrenia in 2020. She took the responsibility to take care her mother-in-law and finished a series of work like recording each prescription, observing her abnormal reactions after the medication, and communication with the doctor. We could see her optimism and strong heart, and a sensitivity in medical problems. She is eager to solve specific problems like investigating the mechanism of mental illness. We believed that her research would be conducive to understanding how to make full use of medical data (physiological electrical signals, medical images), develop new medical devices, and contribute to human health.

To fulfill her goal, she is active to conduct research in computational and applied mathematics. She participated in project 'Registration and 3D reconstruction of serial tissue sections' in cooperation with Sun Yat-sen University Cancer Center from 2021. Her supervisor, Prof. Li Jia in Sun yat-sen University, recognized she made major contribution and largely promoted this project. Besides, she participated in Contemporary Undergraduate Mathematical Contest in Modeling in 2019 and did a followed-up study on 'Data Analysis on the Fairness of Short-trip Taxi Services in Guangzhou Baiyun International Airport'. As a co-first author, Her work is published in the Competition Forum column in Mathematical Modeling and Its Applications, which is a Chinese Journal focusing on mathematical modeling competitions. She showed strong ability in literature search and organization, building models and programming.

In her research plan on Partially coherent Ptychography, she clearly convey the background, objectives, methods, and prior work. Ptychography is a popular imaging technique in scientific fields like condensed matter physics, cell biology, materials science, and electronics, etc. Partial coherence analysis could benefit

high-resolution reconstruction of the specimen from the sequence of intensity measurements under broad experiment condition.