3D Phaseless Imaging at Nano-scale: Challenges and Possible Solutions

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Abstract—**In a variety of scientific applications we are interested in imaging 3D objects at very fine resolutions. However, we typically can not measure the object or its footprint directly. Rather restricted by fundamental laws governing the propagation of light we have access to 2D magnitude-only measurements of the 3D object through highly nonlinear projection mappings. Therefore, reconstructing the object requires inverting highly nonlinear and seemingly non-invertible mappings. In this paper we discuss some of the challenges that arises in such three dimensional phaseless imaging problems and offer possible solutions for 3D reconstruction. In particular we demonstrate how variants of the recently proposed Accelerated Wirtinger Flow (AWF) algorithm can enable precise 3D reconstruction at unprecedented resolutions. This extended abstract is based on a summary of [2], [46], and forthcoming work by the author and collaborators with parts of the text directly adapted.**

I. INTRODUCTION

The ability to image objects at nm scales is of fundamental importance in a variety of scientific and engineering disciplines. For instance, successful imaging of large protein complexes and biological specimens at very fine scales may enable live imaging of biochemical behavior at the molecular level providing new insights. Similarly, modern multilayered integrated circuits increasingly contain features below 10nm in size. The ability to image such specimens non-destructively can be used to improve quality control during the manufacturing process.

Imaging at finer and finer resolutions necessitates shorter and shorter beam wavelengths. However, lens-like devices and other optical components are difficult to build at very short wavelengths. Phase-less coherent diffraction imaging techniques offer an alternative method for recovery of high resolution images without the need for involved measurement setups that include mirrors and lenses. Invention of new light sources and new experimental setups that enable recording and reconstruction of non-crystalline objects has caused a major revival in the use of phase-less imaging techniques [1], [9], [11], [14], [21], [24]–[27], [30], [31], [44], [45]. More recently, successful experiments using ptychography [12], [13], [17], [29], [32], [36], Fourier ptychography [10], [18], [38], [39], [43], [48] and partially coherent ptychography [8] have further contributed to this surge. There has also been tremendous progress in the development of phase retrieval methods with the introduction of new algorithmic approaches that include maximum-likelihood estimation [37], Ptychographic Iterative Engine (PIE) [28] and extended Ptychographic Iterative Engine (ePIE) [22], Difference Map (DM) [35], [36], new variants of the classic Error Reduction (ER) algorithm [47], Relaxed Averaged Alternating Reflections (RAAR) [23], semidefinite programming [3], [4], [6], [19], Wirtinger Flow (WF) [5], proximal algorithms [16], [34], [42], and majorize-minimize methods [41]. See also [7], [20], [33], [40] and references therein for many interesting works on first-order methods and/or theoretical analysis with random sensing ensembles. Despite all of this major progress three dimensional phaseless imaging at nano-scale has remained elusive.

II. 3D PHASELESS IMAGING: MODELS AND CHALLENGES

In this section we discuss a mathematical formulation of the problem by explaining the forward model from the 3D object to the measurements. This exposition is based on [15]. To begin let $\boldsymbol{x}$ denote a three dimensional array representing the complex refractive index of the 3D object. Then the two-dimensional measurements can be written in the form

$$\boldsymbol{y}_\ell = |\boldsymbol{A}\boldsymbol{g}_\ell(\boldsymbol{x})| \quad \text{for} \quad \ell = 1, 2, \ldots, L.$$

Here, ℓ denotes the index of the illumination angle taking values in $\{1, 2, \ldots, L\}$, m is the total number of intensity measurements for all the L angles, $\boldsymbol{y}_\ell \in \mathbb{R}^{\frac{m}{L}}$ is the vector of the square root of the intensity measurement corresponding to angle ℓ, $\boldsymbol{A} \in \mathbb{R}^{\frac{m}{L} \times \frac{m}{L}}$ represents the 2D Fourirer transform and application of the probe function, and $\boldsymbol{g}_\ell(\boldsymbol{x}) \in \mathbb{R}^{\frac{m}{L}}$ denotes the known exit wave corresponding to the projection angle ℓ. At nano-scale, the exit wave $\boldsymbol{g}_\ell$ is a highly nonlinear function that maps the three dimensional object to the two dimensional wave at illumination angle ℓ. The goal is to reconstruct the object $\boldsymbol{x}$ from such observations.

There are many challenges that arise in such 3D phase retrieval problems. First, the forward mapping is highly nonlinear and inverting this nonlinearity requires solving highly nonconvex optimization problems with many local optima. Second, the model maps an inherently three dimensional object in two dimensions introducing many new ambiguities in the reconstruction. For instance, in this problem in addition to the global phase ambiguity common in 2D phase retrieval problem one has to deal with notorious phase wrapping ambiguities that typically occur in tomography. Third, due to the highly complicated nature of the experimental setup a variety of new noise/misalignment effects corrupt the measurements. Finally, acquisition at such fine resolution is extremely slow. For instance imaging a $1cm \times 1cm$ object at $10nm$ can take more than 2500 days.

III. Object Reconstruction via Accelerated Wirtinger Flows

To overcome the challenges discussed in the previous section we formulate the reconstruction problem via the following nonconvex optimization problem

$$\min_{\boldsymbol{z}} \mathcal{L}(\boldsymbol{z}) := \sum_{\ell=1}^{L} \left\| \boldsymbol{y}_\ell - |\boldsymbol{A}\boldsymbol{g}_\ell(\boldsymbol{z})| \right\|_{\ell_2}^2 . \qquad \text{(III.1)}$$

To solve this nonconvex optimization problem and in particular circumvent its highly nonconvex landscape we use a variant of the Accelarated Wirtinger Flow algorithm [46] which utilizes Nesterov-style acceleration to circumvent local optima. In particular, theoretical results enable prespecification of all AWF algorithm parameters, with no need for computationally-expensive line searches and no need for manual parameter tuning. Furthemore, we develop a variety of heuristics to deal with the aforementioned ambiguity factors (see the presentation accompanying this paper for more detail). Finally, to reduce the acquisition time we use a regularized variant of the formulation above where we utilize training data to learn the appropriate regularizer for a given reconstruction task. In the presentation accompanying this paper we demonstrate the effectiveness of our approach for 3D reconstruction of a variety of nanostructures.

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