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Alternating projection, ptychographic imaging and phase synchronization

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A B S T R A C T

We demonstrate necessary and sufficient conditions of the local convergence of the alternating projection algorithm to a unique solution up to a global phase factor. Additionally, for the ptychography imaging problem, we discuss phase synchronization and graph connection Laplacian, and show how to construct an accurate initial guess to accelerate convergence speed to handle the big imaging data in the coming new light source era.

1. Introduction

The reconstruction of a scattering potential from measurements of scattered intensity in the "far-field" has occupied scientists and applied mathematicians for over a century, and arises in fields as varied as optics [34,51], astronomy [35], X-ray crystallography [28], tomographic imaging [57], holography [22,54], electron microscopy [42] and particle scattering generally. Although phase-less diffraction measurements using short wavelength (such as X-ray, neutron, or electron wave packets) have been at the foundation of some of the most dramatic breakthrough in science – such as the first direct confirmation of the existence of atoms [11,12], the structure of DNA [71], RNA [25] and over 100,000 proteins or drugs involved in human life [9,47] – the solution to the scattering problem for a general object was generally thought to be impossible for many years. Nevertheless, numerous experimental techniques that employ forms of interferometric/holographic [22,54] measurements, gratings [61], and other phase mechanisms like random phase masks, sparsity structure, etc.

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[1,4,16,15,69,32,70,3] to help overcome the problem of phase-less measurements have been proposed over the years [59,31,40].

More recently an experimental technique has emerged that enables to image what no one was able to see before: macroscopic specimens in 3D at wavelength (i.e. potentially atomic) resolution, with chemical state specificity. Ptychography was proposed in 1969 [45,44,58,18,62] to improve the resolution in electron or X-ray microscopy by combining microscopy with scattering measurements. This technique enables one to build up very large images at wavelength resolution by combining the large field of view of a high precision scanning microscope system with the resolution enabled by diffraction measurements. In other words, the diffractive imaging and the scanning microscope techniques are combined together.

Initially, technological problems made ptychography impractical. Now, thanks to advances in source brightness [19,10] and detector speed [13,27], research institutions around the world are rushing to develop hundreds of ptychographic microscopes to help scientists understand ever more complex nano-materials, self-assembled devices, or to study different length-scales involved in life, from macro-molecular machines to bones [26], and whenever observing the whole picture is as important as recovering local atomic arrangement of the components.

Experimentally, ptychography works by retrofitting a scanning microscope with a parallel detector. In a scanning microscope, a small beam is focused onto the sample via a lens, and the transmission is measured in a single-element detector. The image is built up by plotting the transmission as a function of the sample position as it is rastered across the beam. In such microscope, the resolution of the image is given by the beam size. In ptychography, one replaces the single element detector with a two-dimensional array detector such as a CCD and measures the intensity distribution at many scattering angles, much like a radar detector system for the microscopic world. Each recorded diffraction pattern contains short-spatial Fourier frequency information [38] about features that are smaller than the beam-size, enabling higher resolution. At short wavelengths however it is only possible to measure the intensity of the diffracted light. To reconstruct an image of the object, one needs to retrieve the phase. The phase retrieval problem is made tractable in ptychography by recording multiple diffraction patterns from the same region of the object, compensating phase-less information with a redundant set of measurements.

While reconstruction methods often work well in practice, fundamental mathematical questions concerning their convergence remain unresolved. The reader of an experimental paper is often left to wonder if the image and the resulting claims are valid, or one possibility among many solutions. Retractions of experimental results do happen (see [66] for a discussion of controversial results in the optical community), and the problem is exacerbated because reproducing an image a nanoscale object is often not practical. What are often referred to as convergence results for projection algorithms are far from what we need for global convergence [51].

A popular algorithm for solving the phase retrieval problem was proposed in 1972. In their famous paper, Gerchberg and Saxton [37], independently of previous mathematical results for projections onto convex sets, proposed a simple algorithm for solving phase retrieval problems in two dimensions. In [48] the algorithm was recognized as a projection algorithm that involves alternating projections between measurement space and object space. In 1982 Fienup [34] generalized the Gerchberg–Saxton algorithm and analyzed many of its properties, showing, in particular, that the directions of the projections in the generalized Gerchberg–Saxton algorithm are formally similar to directions of steepest descent for a distance metric. One particular algorithm we focus on this paper is the alternating projection (AP) algorithm, which iteratively alternates between enforcing two pieces of information about the phase retrieval problem: the solution has known measured amplitude, and the illumination geometry is known. The main purpose of the AP algorithm is finding the solution that satisfies both conditions simultaneously.

Projection algorithms for convex sets have been well understood since 1960s. The phase retrieval problem, however, involves nonconvex sets. For this reason, the convergence properties of the Gerchberg–Saxton algorithm and its variants is still an open question except in very special cases [51,49].