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Fourier phase retrieval with a single mask by Douglas–Rachford algorithms

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ABSTRACT

The Fourier-domain Douglas–Rachford (FDR) algorithm is analyzed for phase retrieval with a single random mask. Since the uniqueness of phase retrieval solution requires more than a single oversampled coded diffraction pattern, the extra information is imposed in either of the following forms: 1) the sector condition on the object; 2) another oversampled diffraction pattern, coded or uncoded.

For both settings, the uniqueness of projected fixed point is proved and for setting 2) the local, geometric convergence is derived with a rate given by a spectral gap condition. Numerical experiments demonstrate global, power-law convergence of FDR from arbitrary initialization for both settings as well as for 3 or more coded diffraction patterns *without* oversampling. In practice, the geometric convergence can be recovered from the power-law regime by a simple projection trick, resulting in highly accurate reconstruction from generic initialization.

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1. Introduction

X-ray crystallography has been the preferred technology for determining the structure of a biological molecule over the past hundred years. The method, however, is limited by crystal quality, radiation damage and phase determination [44,48]. The first two problems call for large crystals that yield sufficient diffraction intensities while reducing the dose to individual molecules in the crystal. The difficulty of growing large, well-diffracting crystals is thus the major bottleneck of X-ray crystallography – a necessary experimental step that can range from merely challenging to pretty much impossible, particularly for large macromolecular assemblies and membrane proteins.

By boosting the brightness of available X-rays by 10 orders of magnitude and producing pulses well below 100 fs duration, X-ray free electron lasers (XFEL) offer the possibility of extending structural studies to *single, non-crystalline* particles or molecules by using short intense pulses that out-run radiation damage,

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thus circumventing the first two aforementioned problems [50]. In the so-called *diffract-before-destruct* approach [20,21,56], a stream of particles is flowed across the XFEL beam and randomly hit by a single X-ray pulse, forming a single diffraction pattern before being vaporized as a nano-plasma burst. Each diffraction pattern contains certain information about the planar projection of the scatterer along the direction of the beam which is to be recovered by phase retrieval techniques [11].

The modern approach to phase retrieval for non-periodic objects roughly starts with the Gerchberg–Saxton algorithm [34], followed by its variant, Error Reduction (ER), and the more powerful Hybrid-Input–Output (HIO) algorithm [32,33]. These form the cornerstones of the standard *iterative transform algorithms* (ITA) [8,43].

However, the standard ITA tend to stagnate and do not perform well without additional prior information, such as tight support and positivity. The reason is that the *plain* diffraction pattern alone does not guarantee uniqueness of solution (see [54], however, for uniqueness under additional prior information). On the contrary, many phase retrieval solutions exist for a given diffraction pattern, resulting in what is called the *phase* problem [37].

To this end, a promising approach is to measure the diffraction pattern with a *single* random mask and use the coded diffraction pattern as the data. As shown in [28], the uniqueness of solution is restored with a high probability given any scatterer whose value is restricted to a known sector (say, the upper half plane) of the complex plane (see Proposition 2.1).

Indeed, the sector constraint is a practical, realistic condition to impose on almost all materials as the imaginary part of the scatterer is proportional to the (positive) extinction coefficient with the upper half plane as the sector constraint [11]. For X-ray, the scatterers usually have positive real (except for resonance frequencies) and imaginary parts, making the first quadrant the sector constraint [18].

What happens if the sector condition is not met and consequently one coded diffraction pattern is not enough to ensure uniqueness? This question is particularly pertinent to the diffract-before-destruct approach as the particle can not withstand the radiation damage from more than one XFEL pulses.

A plausible measurement scheme is to guide the transmitted field (the transmission function [11]) from a *planar* illumination through a beam splitter [52], generating two copies of the transmitted field which are then measured separately as a coded diffraction pattern and a plain diffraction pattern. In this set-up, the object function is the transmitted field behind the particle and the phase retrieval problem becomes the wave-front reconstruction problem [11,36]. In practice beam splitters and the masks (or any measurement devices) should be used as sparingly as possible to avoid introducing excessive noises in the data.

As shown in [28], phase retrieval with two coded diffraction patterns has a unique solution, up to a constant phase factor, almost surely without the sector constraint (see Proposition 2.1).

With the uniqueness-ensuring sampling schemes (Section 1.1), *ad hoc* combinations of members of ITA (such as HIO and ER) can be devised to recover the true solution [30,31]. There is, however, no convergence proof for these algorithms, except for alternating projections, including ER (see [22] and references therein).

The main goal of the paper is to prove the *local, geometric convergence* of the Douglas–Rachford (DR) algorithm to a unique fixed point in the case of one or two oversampled diffraction patterns (Theorems 5.1, 6.3 and 4.2) and demonstrate *global convergence* numerically (Section 7).

DR has the following general form: Let P_1 and P_2 be the projections onto the two constraint sets, respectively. For phase retrieval, P_1 describes the projection onto the set of diffracted *fields* and P_2 the data fitting projector constrained by the measured diffraction patterns. Let $R_1 = 2P_1 - I$ and $R_2 = 2P_2 - I$ be the respective reflection operators. The Douglas–Rachford (DR) algorithm is defined by the *average alternating reflection* scheme [24,25,41]

$$\begin{aligned} y^{(k+1)} &:= \frac{1}{2}(I + R_1R_2)y^{(k)} \\ &= y^{(k)} + P_1(2P_2 - I)y^{(k)} - P_2y^{(k)}, \quad k = 1, 2, 3 \cdots \end{aligned} \tag{1}$$

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