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Phase retrieval from diffraction data utilizing pre-determined partial information

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Abstract

We developed a phase retrieval algorithm that utilizes pre-determined partial phase information to overcome insufficient oversampling ratio in diffraction data. Implementing the Fourier modulus projection and the modified support projection manifesting the pre-determined information, a generalized difference map and HIO (Hybrid Input–Output) algorithms are developed. Optical laser diffraction data as well as simulated X-ray diffraction data are used to illustrate the validity of the proposed algorithm, which revealed the strength and the limitations of the algorithm. The proposed algorithm can expand the applicability of the diffraction based image reconstruction.

Keywords: Phase retrieval; Oversampling; X-ray imaging

1. Introduction

In most diffraction measurements, such as X-ray, electron, and neutron diffraction, phase retrieval has been one of the most challenging problems [1–6]. Since only the Fourier modulus is measured in typical diffraction experiments, the phase information is lost, and additional a priori information is required to retrieve the phase or to reconstruct a real space image. Recently various oversampling methods have been suggested and successfully applied to retrieve the phase information in case of non-crystalline objects. The first successful iterative algorithm was proposed by Gerchberg and Saxton [7], in which modulus constraints in real object domain and Fourier domain are applied in alternating order. This algorithm was modified by Fienup, who developed an error reduction algorithm which utilized the support constraint rather than the modulus constraint in object domain [8]. To overcome the stagnation problems inherent to the Fienup's original algorithm, Fienup further developed a hybrid input–output(HIO) algorithm adopting ideas used in control theories [9,10]. HIO method is one of the most powerful and widely used algorithms in imaging reconstruction from diffraction. Later, Elser developed a difference map routine which is composed of the difference of a pair of elementary projections [11–13]. The formalism used in the difference map is so general and flexible that the HIO method can be considered as a special case of the difference map.

In this paper we present an iterative phase retrieval method that is applicable to reconstruct an image using pre-determined partial information of the non-periodic object as a priori information. The constraint of zero-density outside the support area, which is typical constraint used in conventional HIO algorithms, is replaced by the constraint of predetermined density in part of the object area. The proposed generalized difference map algorithm is based on the generalized support projection as discussed in Section 2. The proposed algorithm was tested by reconstructing images from simulated X-ray diffraction data. It is shown that an electron density can be reconstructed from diffraction data even in the cases where oversampling ratio less than 2. Furthermore, optical diffraction data obtained using an He–Ne laser under various constraints were used to test the algorithm. The results of the laser experiment illustrate the strength and the weakness of the proposed algorithm.

2. Phase retrieval algorithm based on pre-determined information

In this section, we present a phase retrieval algorithm that is applicable to a system whose partial electron density information is available. The key idea is to utilize the pre-determined partial information to overcome insufficient oversampling ratio.

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We first introduce the conventional difference map algorithm, a procedure of reconstructing electron density from measured Fourier modulus generally applicable to diffraction data obtained under sufficient oversampling ratio [11–13]. The object is to find a solution (electron density) $\rho_S(\vec{r})$ which is consistent with the measured Fourier modulus $|F[\rho_S(\vec{r})]|$, and a given support constraint, $\rho_S(\vec{r}) = 0$ for all $\vec{r} \notin S$, where S represents a support of non-zero density area. The ratio of the total area to the support area S defines the oversampling ratio, which is generally required to be greater than 2.

In most algorithms, two important projections are defined which are the Fourier modulus and the support projections respectively. The Fourier modulus projection is defined as, $\Pi_F[\rho(\vec{r})] = F^{-1} \circ \tilde{\Pi}_F \circ F[\rho(\vec{r})]$, where F is a unitary Fourier transform and $\tilde{\Pi}_F$ is an operator which replace the modulus of $F[\rho(\vec{r})]$ by the measured modulus while leaving the phase unchanged. $\Pi_F[\rho(\vec{r})]$ finds a density whose Fourier phase is the same as $\rho(\vec{r})$, but Fourier modulus is replaced by the measured modulus. The support projection Π_S, which places a constraint in real space, is defined as,

$$\Pi_S[\rho(\vec{r})] = \begin{cases} \rho(\vec{r}) & \text{for } r \in S \\ 0 & \text{otherwise} \end{cases}. \tag{1}$$

In iterative phase retrieval algorithms, S represents an unknown density region while compliment of S is known density region. In a standard support projection, density in compliment of S has zero value. In most reported algorithms, starting from a random initial density, Π_F and Π_S are iteratively applied to the outcomes to find a true solution.

In the difference map algorithm, to improve the stagnation problem, a difference operator is defined as [11],

$$\Delta = \Pi_S \circ [(1+\gamma_2)\Pi_F - \gamma_2] - \Pi_F \circ [(1+\gamma_1)\Pi_S - \gamma_1], \tag{2}$$

where γ_1 and γ_2 are real numbers of order 1. With the difference operator, the difference map in each iteration is defined as $\vec{\rho}_{n+1} = \vec{\rho}_n + \beta \Delta \vec{\rho}_n$, where β is a real number. The strength of the difference map is the generality of the algorithm. By selecting appropriate values of γ_1 and γ_2, one may reconstruct electron densities in various situations.

The major idea of the proposed algorithm using predetermined information is to replace the density in the complimentary region of S from zero density to the predetermined density. Assuming compliment of S has $K(\vec{r})$, we can define general support projection $\Pi_S^{\vec{K}}$ as follows

$$\Pi_S^{\vec{K}}[\rho(\vec{r})] = \begin{cases} \rho(\vec{r}) & \text{for } r \in S \\ K(\vec{r}) & \text{otherwise} \end{cases}. \tag{3}$$

It can be verified that subspace formed by above constraint is convex and $\Pi_S^{\vec{K}}$ is an elementary projection operator to that subspace. For $K(\vec{r}) = 0$, $\Pi_S^{\vec{K}}$ or Π_S^0 is reduced to the standard support projection, Π_S. Thus, $\Pi_S^{\vec{K}}$ can be considered as a general form of support projection, Π_S. The difference operator Δ is then modified to

$$\Delta = \Pi_S^{\vec{K}} \circ [(1+\gamma_2)\Pi_F - \gamma_2] - \Pi_F \circ [(1+\gamma_1)\Pi_S^{\vec{K}} - \gamma_1]. \tag{4}$$

With $\gamma_1 = -1$ and $\gamma_2 = \beta^{-1}$ in Eq. (4), we can also construct a corresponding difference operator for the HIO algorithm [11],

$$\Delta_{\mathrm{HIO}} = \Pi_S^{\vec{K}} \circ [(1+\beta^{-1})\Pi_F - \beta^{-1}] - \Pi_F. \tag{5}$$

By applying Δ_{HIO}, we can get the final HIO iteration routine,

$$\vec{\rho}_{n+1}(r) = \begin{cases} \Pi_F[\vec{\rho}_n(r)] & r \in S \\ \vec{\rho}_n(r) + \beta\{\vec{K}(r) - \Pi_F[\vec{\rho}_n(r)]\} & r \notin S \end{cases}, \tag{6}$$

where the support S is a unknown density region and $\vec{K}(r)$ is a pre-determined density in the compliment of S. If we choose dynamic support S by calculating autocorrelation function of the result in each iteration, we can also get the modified shrink-wrap algorithm [14].

3. Reconstruction of electron density from simulated X-ray diffraction data

To verify the applicability of the proposed algorithm based on predetermined partial information, we performed computer simulations on phasing experiments. Since the ultimate applications for the algorithm is reconstructing images from coherent X-ray diffraction data, we simulated the diffraction pattern of an Au pattern of 250 nm thick under X-rays of $\lambda = 2$ Å.

The simulation was carried out in the following steps. First, we calculated the electron density of the initial configuration which is composed of an outer zero-density area and an inner nonzero-density area as shown in Fig. 1(a) We fixed the oversampling ratio, the ratio of the total area to non-zero to 5.8. Fig. 1(b) shows the simulated X-ray diffraction pattern. Second, we calculated the electron density of the target configuration shown in Fig. 1(c). The central part of the target configuration is the same as the initial configuration but the zero-density area is reduced. The oversampling ratio is 1.9, less than 2 in this case. The simulated diffraction pattern of the target configuration is shown in Fig. 1(d).

Using the simulated diffraction pattern, Fig. 1 (b) and (d), we applied the proposed algorithm to reconstruct the target image. First, we reconstructed the electron density of the initial configuration applying the HIO algorithm and the difference map. Since the oversampling ratio is larger than 2, the image reconstruction was straightforward. Next, using the diffraction pattern of the target configuration shown in Fig. 1(d), and the reconstructed electron density of the initial configuration, we reconstructed the target electron density. The result of the reconstruction using the HIO algorithm and the initial density reconstructed by the HIO algorithm (HIO–HIO combination) is shown in Fig. 1(e). The reconstructed image using the difference map with the initial density reconstructed also by the difference map (difference–difference combination) is shown in Fig. 1(f). Random phase set was used as an initial condition with reconstruction parameters, $\beta_{\mathrm{HIO}} = 0.8$, $\beta_{\mathrm{DIF}} = 1.0$, $\gamma_1 = -1.0$ and $\gamma_2 = 1.0$ respectively. The number of iterations was less than 500 in all cases.