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Invited Paper

An Information-Theoretic Approach to Phase Retrieval

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Abstract

Phase problems arise from the lost Fourier phase in measuring the diffraction waves. Reconstructing the phase information using the diffraction pattern of a target object yields the target image, and it is called *phase retrieval.* This paper introduces an information-theoretic approach to phase retrieval based on information measures, and a refined derivation of the generalized phase retrieval algorithm based on the density power divergence is presented with a simple numerical example using the Poisson-noise-contaminated Fourier intensity.

Keywords: Phase Retrieval, Information Divergence, Iterative Algorithm.

1. Introduction

Losing the Fourier phase in measuring the diffraction waves is called "*phase problems*" in a diverse field of physics; x-ray crystallography, x-ray and electron microscopies, astronomy, and general optics. The recent related topics are in the reference [16]. As a mathematical representation of the problems, let ρ be the target object, and the intensity measurement of the Fourier transformed ρ is given. The objective is to reconstruct the Fourier phase.

The phase retrieval is to reconstruct the missing phase in the Fourier domain while the intensity measurements are observed. The possibility to retrieve the lost phase

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was first pointed out by Sayer [15] in terms of Shannon's sampling theorem. A cyclic diagram using the Fourier transforms for phase retrieval was presented by Gerchberg and Saxton [5]. And then, Fienup presented an error reduction (ER) algorithm based on the steepest-descent method and the hybrid input-output (HIO) algorithm [4]. These algorithms have been used in the fields of astronomy, general optics, x-ray crystallography and electron microscopy. Experimental results of imaging from the diffraction pattern without an objective lens using various light sources have been presented; imaging using x-ray diffraction pattern [9, 10, 11, 13, 3], electron microscope [23, 6, 12], and tabletop light sources of lasers [14]. Imaging without lens has been represented as *diffractive imaging* [21].

Concerning the theoretical research for phase retrieval, a generalized phase retrieval algorithm based on information measures was presented by Shioya and Gohara [17]. Their result reveals that the ER algorithm is a kind of generalized phase retrieval algorithm based on the density power divergence [1, 22]. And also, a new iterative phase retrieval based on the maximum entropy method for the diffractive imaging was introduced [18]. In this paper, we introduce an information-theoretic approach to phase retrieval with a refined derivation of the generalized phase retrieval algorithm, and a simple numerical example of phase retrieval is presented using the Poisson-noise-contaminated Fourier intensity.

2. Phase Retrieval

Measuring the diffraction wave from a target object, the diffraction patten consisted by the intensity are measured, but the Fourier phase is lost. Losing the Fourier phase in the measurement is called *phase problem*. The reconstruction of the phase is called *phase retrieval*. In crystallography, the x-ray diffraction patterns of crystallines give the structures of periodic materials, however, it is difficult to reconstruct the lost Fourier phase in the case of non-periodic materials.

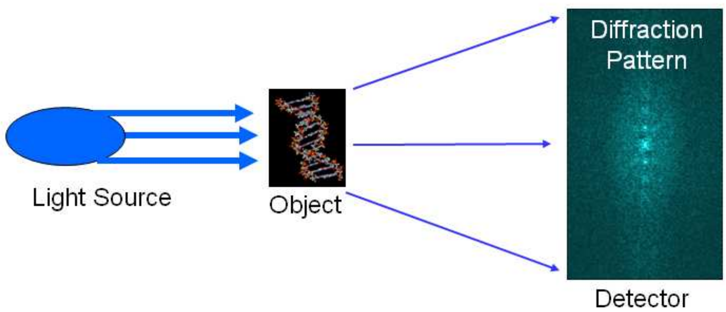

Figure 1: The relationship between the objects and diffraction patterns.

Figure 1 presents the relationship between an object and its diffraction pattern. Based on the figure, let ρ be the object as the target material, and let S be the domain defining the object function ρ. Let the domain S be a discrete square array, $N \times N$ ($N \in \mathbb{N}$). The diffraction waves form ρ at the detector are presented by the following discrete Fourier transform of ρ.

$$F_\rho(k) = \sum_{\boldsymbol{r} \in S} \rho(\boldsymbol{r}) \exp\{-i2\pi \boldsymbol{k} \cdot \boldsymbol{r}/N\}. \tag{1}$$

where k is an index of the Fourier domain K $(= N \times N)$. The observed data at the detector is the intensity data, and the phase is lost. If we have an estimation of the lost phase, $\hat{\psi}(\boldsymbol{k})$, we have $\hat{F}(\boldsymbol{k}) = |F_{\text{obs}}(k)| \exp(i\hat{\psi}(\boldsymbol{k}))$ and the following inverse Fourier transform gives an estimation, $\hat{\rho}(\boldsymbol{r})$.

$$\hat{\rho}(\boldsymbol{r}) = \frac{1}{N^2} \sum_{\boldsymbol{k} \in K} \hat{F}(\boldsymbol{k}) \exp\{i2\pi \boldsymbol{k} \cdot \boldsymbol{r}/N\}. \tag{2}$$

As a practical method for phase retrieval, the algorithm consisted by the iterative Fourier transforms was presented by Gerchberg and Saxton [5]. Their cyclic diagram is presented in Fig. 2. The procedure of their algorithm is described as follows. The prior object ρ is transformed into F by the Fourier transform FT; F is replaced by F' (the amplitude is given by the experiment in the Fourier domain, and the phase of F' is the same as that of F, while the replaced amplitude is the constraint in the Fourier domain); ρ' is obtained by the inverse Fourier transform of F'; and ρ' is replaced by the updated object as the next ρ using some constraints in the object domain. And, Fienup presented

$$\begin{tikzcd} \rho \arrow[r, "\text{FT}"] & F \arrow[d] \\ \rho' \arrow[u] & F' \arrow[l, "\text{Inverse FT}"'] \end{tikzcd}$$

Figure 2: Gerchberg-Saxton diagram for phase retrieval.

the error reduction (ER) algorithm and the hybrid input output (HIO) algorithm with computer simulations [4]. The ER is described as

$$\rho_{n+1}(\boldsymbol{r}) = \begin{cases} \rho'_n(\boldsymbol{r}) & \boldsymbol{r} \notin \bar{S} \\ 0 & \boldsymbol{r} \in \bar{S} \end{cases}, \tag{3}$$

where $\bar{S}$ is the set of points at which ρ'_n violates the object-domain constraints. The following is the HIO, which is an improved version of the updating method with respect to the region breaking the object-domain constraints:

$$\rho_{n+1}(\boldsymbol{r}) = \begin{cases} \rho'_n(\boldsymbol{r}) & \boldsymbol{r} \notin \bar{S} \\ \rho_n(\boldsymbol{r}) - \beta\rho'_n(\boldsymbol{r}) & \boldsymbol{r} \in \bar{S} \end{cases}, \tag{4}$$

where β is a positive constant. Although the Fourier phase was lost, the goodness of the estimated phase can not be evaluated. Then, using the Fourier transform of the estimated object $\hat{\rho}$ obtained by the phase, the following R-factor is well-used.

$$R(\hat{F}, F_{\mathrm{obs}}) = \frac{\sum_{\boldsymbol{k}\in K} ||\hat{F}(\boldsymbol{k})| - |F_{\mathrm{obs}}(\boldsymbol{k})||}{\sum_{\boldsymbol{k}\in K} |F_{\mathrm{obs}}(\boldsymbol{k})|}. \tag{5}$$

The ER and HIO are regarded as identical with respect to the updating at points satisfying the object-domain constraints. These algorithms have been effectively used for the non-periodic case. However, the analysis of retrieving the lost phase for the case are not still sufficient to reveal the pure theoretical aspect of phase retrieval. Then, an advance analysis of phase retrieval based on an information-theoretic approach is needed.

3. Information-Based Analysis for Phase Retrieval

In this section, we describe the problem for phase retrieval in terms of information divergences. Based on the iterative algorithms for phase retrieval using a generalized information divergence [17], we present a refined derivation of the algorithms.

The problem is to estimate unknown object using the object and Fourier domain constraints. Let ρ_{target} be the target function on the domain S, where $\rho(x) \in \mathbb{C}, x \in S$. Two constraints are given in this problem. One is the Fourier intensity of ρ_{target}, $|\mathrm{FT}(\rho_{\mathrm{target}})|$, as the Fourier-domain constraint. Another is the prior information of the target as the object-domain constraint. The problem is to reconstruct the reconstruction of the phase of $\mathrm{FT}(\rho_{\mathrm{target}})$.

We then define the following finite-norm function sets, $\mathbb{S}$ and $\mathbb{K}$.

$$\mathbb{S} = \{\rho \mid \sum_{\boldsymbol{r}\in S} |\rho(\boldsymbol{r})| < \infty\}, \tag{6}$$

$$\mathbb{K} = \{F \mid \sum_{\boldsymbol{k}\in K} |F(\boldsymbol{k})| < \infty\}. \tag{7}$$

More over, using L^1-norm, the function spaces, $\mathbb{F}_{\mathrm{obj}} = (\mathbb{S}, L^1)$ and $\mathbb{F}_{\mathrm{Fourier}} = (\mathbb{K}, L^1)$, are introduced. Using the two function spaces, we have a new representation of the GS-diagram shown in Fig 3. As the Fourier-domain constraint, $|F_{\mathrm{obs}}|^2$ is given, and the object-domain constraint is given as prior information of the target object on the object domain. Then, let $\mathrm{S}_{\mathrm{obj}}$ be a subset of $\mathbb{S}$ satisfying the object-domain constraints, and $\mathrm{S}_{\mathrm{obs}}$ is a subset of $\mathbb{S}$ satisfying the Fourier-domain constraint given by $|F_{\mathrm{obs}}|^2$. Let us define the following pair given by the minimization of the L^1-distance between an element of $\mathrm{S}_{\mathrm{obj}}$ and that of $\mathrm{S}_{\mathrm{obs}}$. This gives a plausible object, ρ_{obj}, regarded as a phase-retrieved object.

$$(\rho_{\mathrm{obs}}, \rho_{\mathrm{obj}}) = \arg\min_{\rho_1\in \mathrm{S}_{\mathrm{obs}}, \rho_2 \in \mathrm{S}_{\mathrm{obj}}} L(\rho_1, \rho_2), \tag{8}$$

where $\rho_{\mathrm{obs}} \in \mathrm{S}_{\mathrm{obs}}$, $\rho_{\mathrm{obj}} \in \mathrm{S}_{\mathrm{obj}}$, and $L(\rho_1, \rho_2) = \|\rho_1 - \rho_2\|$.

If $\mathrm{S}_{\mathrm{obj}} \cap \mathrm{S}_{\mathrm{obs}} \neq \phi$, there exists ρ_{obj} satisfying $\rho_{\mathrm{obj}} = \rho_{\mathrm{obs}}$. If the cardinality of $\mathrm{S}_{\mathrm{obj}} \cap \mathrm{S}_{\mathrm{obs}}$ is greater than 1, the solution of this problem is not unique. If $\mathrm{S}_{\mathrm{obj}} \cap \mathrm{S}_{\mathrm{obs}}$ is

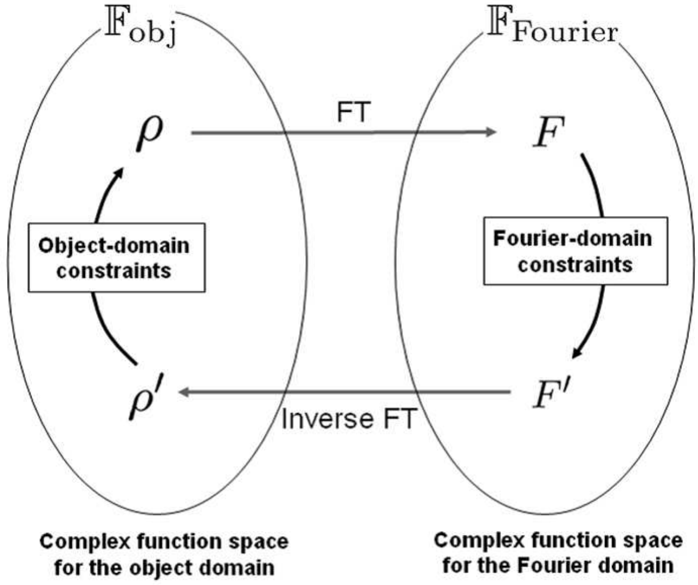

Figure 3: Coming and going between two function spaces $\mathbb{F}_{\text{obs}}$ and $\mathbb{F}_{\text{Fourier}}$ by the Fourier transformation.

empty, these is no object perfectly satisfying both constraints. Therefore, ρ_{obj} is a least favorable estimation not satisfying the Fourier-domain constraint given as the observed $|F_{\text{obj}}|$. The pair $(\rho_{\text{obs}}, \rho_{\text{obj}})$ is related to the pair (ρ', ρ) obtained by sufficiently-iterated original GS-diagram (Fig. 2) with the ER algorithm, and the object support as the object-domain constraints. Then, we present the relationship between an information-theoretic method and phase retrieval in the next.

We suppose that ρ and ρ' are real and non-negative functions, and define the information discriminant measures as follows.

$$D_2(\rho, \rho') = \sum_{\boldsymbol{r} \in S} \{\rho(\boldsymbol{r}) - \rho'(\boldsymbol{r})\}^2. \tag{9}$$

$$D_2(F, F') = \sum_{\boldsymbol{k} \in K} |F(\boldsymbol{k}) - F'(\boldsymbol{k})|^2. \tag{10}$$

The phase of F' is same as that of F because of the Fourier domain constraint. Then we have

$$D_2(F, F') = D_2(|F|, |F'|). \tag{11}$$

Here, in order to introduce the update rule of the object functions for phase retrieval, let us define ρ and τ as the prior and posterior objects, respectively. Figure 4 presents two information measures, $D_2(\rho, \tau)$ and $D_2(F, F')$, which are the discriminant measures on object and Fourier function spaces. Using the two information discriminant measures, we introduce the following.

$$\mathcal{L}_2 = D_2(\rho, \tau) + \lambda D_2(F, F'), \tag{12}$$

where $F = |F_\rho| \exp(i\psi_\rho)$ and $F' = |F_{\mathrm{obs}}| \exp(i\psi_\rho)$. Using $\partial \mathcal{L}_2 / \partial \rho = 0$, we have

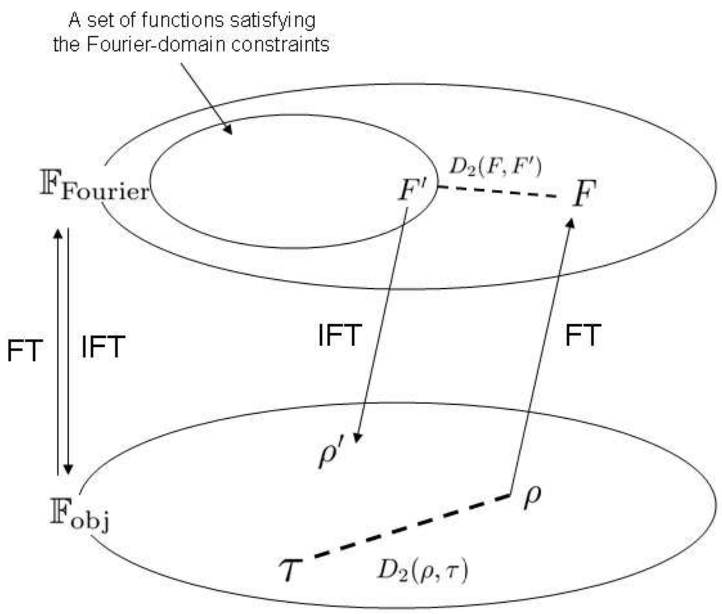

Figure 4: $D_2(\rho, \tau)$ and $D_2(F, F')$ on two connective function spaces, $\mathbb{F}_{\mathrm{obs}}$ and $\mathbb{F}_{\mathrm{Fourier}}$.

$$\rho(\boldsymbol{r}) - \tau(\boldsymbol{r}) + \lambda(\rho(\boldsymbol{r}) - \rho'(\boldsymbol{r})) = 0. \tag{13}$$

However, this does not give an update rule of the ER. In the reference [17], the assumption, that $\|\rho - \tau\|$ is sufficient small, is analytically used. In this paper, we present a refined derivation of the update rules for making the information-theoretic approach clear.

Let us consider the problem minimizing the first term of $\mathcal{L}_2$ and maximizing the second term of $\mathcal{L}$. For the purpose of this change, the following $\bar{\mathcal{L}}_2$ is easily given as

$$\bar{\mathcal{L}}_2 = D_2(\rho, \tau) - \lambda D_2(F, F'). \tag{14}$$

Then, using $\partial \bar{\mathcal{L}}_2 / \partial \rho = 0$, we have

$$\rho(\boldsymbol{r}) - \tau(\boldsymbol{r}) - \lambda(\rho(\boldsymbol{r}) - \rho'(\boldsymbol{r})) = 0. \tag{15}$$

This means that $D_2(\rho, \tau)$ is small and the R-factor is large. The inverse update of Eq. (15) yields the minimization of $\mathcal{L}_2$. Then we have the following update rule from nth object to $(n+1)$th object by

$$\rho_{n+1}(\boldsymbol{r}) = \rho_n(\boldsymbol{r}) - \lambda(\rho_n(\boldsymbol{r}) - \rho'_n(\boldsymbol{r})). \tag{16}$$

In the case of $\lambda = 1$, we have the ER algorithm. Above result gives the relationship between the information discriminant measure D_2 and the ER algorithm. And the assumption, that $\|\rho_n - \rho_{n+1}\|$ is sufficient small, is not needed to derivate Eq. (16).

From the view of generalizing information divergence measures, Shioya and Gohara presented the generalized phase retrieval algorithms [17]. Concretely, they use the following γ-divergence [1, 22] as the first term of $\mathcal{L}_2$.

$$D_\gamma(\rho, \tau) = \sum_{\boldsymbol{r} \in S} \left\{ \frac{1}{\gamma} \rho(\boldsymbol{r})(\rho(\boldsymbol{r})^\gamma - \tau(\boldsymbol{r})^\gamma) - \frac{1}{1+\gamma} \left(\rho(\boldsymbol{r})^{1+\gamma} - \tau(\boldsymbol{r})^{1+\gamma} \right) \right\}, \tag{17}$$

where $\gamma \in [0, 1]$. Some advanced mathematical properties of γ-divergence are in the reference [2]. The Lagrange formula using γ-divergence is given by

$$\mathcal{L}_\gamma = D_\gamma(\rho, \tau) + \lambda D_2(F, F'). \tag{18}$$

Minimizing this Lagrange formula yields the following.

$$\rho(\boldsymbol{r}) = \{\tau(\boldsymbol{r})^\gamma + \lambda\, \gamma(\rho'(\boldsymbol{r}) - \rho(\boldsymbol{r}))\}^{\frac{1}{\gamma}}. \tag{19}$$

However, this does not presented the update rule for ρ only using τ. Then, we change the problem for minimizing the first term of $\mathcal{L}_\gamma$ and for maximizing the second term of $\mathcal{L}_\gamma$. The Lagrange formula of this changed problem is given by

$$\bar{\mathcal{L}}_\gamma = D_\gamma(\rho, \tau) - \lambda D_2(F, F'). \tag{20}$$

The minimization of this gives the following.

$$\rho(\boldsymbol{r}) = \{\tau(\boldsymbol{r})^\gamma - \lambda\, \gamma(\rho'(\boldsymbol{r}) - \rho(\boldsymbol{r}))\}^{\frac{1}{\gamma}}, \tag{21}$$

where $0 \leq \gamma \leq 1$ This gives ρ, which is near by τ in the meaning of γ-divergence and the R-factor is large. The inverse update of Eq. (21) gives the minimization of $\mathcal{L}_\gamma$ as same as in the case of $\mathcal{L}_2$. Then we have the following update rule from nth object to $(n+1)$th object by

$$\rho_{n+1}(\boldsymbol{r}) = \{\rho_n(\boldsymbol{r})^\gamma + \lambda\, \gamma(\rho'_n(\boldsymbol{r}) - \rho_n(\boldsymbol{r}))\}^{\frac{1}{\gamma}}, \tag{22}$$

where $0 \leq \gamma \leq 1$ The case of $\gamma = 0$ gives a typical iterative phase retrieval algorithm based on the maximum entropy method, which is essentially different from usual MEM algorithm for crystallography [18]. Therefore, an information-theoretic approach to phase retrieval gives a new view to phase problem from the field of information theory.

4. Numerical Example

We performed the algorithms ($0 \leq \gamma \leq 1$) in the case using the true Fourier intensity, $|F_{\mathrm{target}}|^2$, of the target object ρ_{target}, and a feasible object is obtained for each case. Therefore, we introduce a numerical example to present the effectiveness of the proposed generalized algorithms for phase-retrieving from the Fourier intensity contaminated by Poisson noise. At the detector in measuring the diffraction waves, the Poisson noise can not be removed from the observed intensity measurement, fundamentally. The Fourier intensity contaminated by Poisson noise is given by

$$|F_{\mathrm{obs}}^{\mathrm{poisson}}(\boldsymbol{k})|^2 \sim c \text{ Poisson}\left(\frac{|F_{\mathrm{target}}(\boldsymbol{k})|^2}{c}\right). \tag{23}$$

where c is the coefficient depending on the total count. The Fourier intensity of the target object, $|F_{\mathrm{target}}|^2$, is used as the expectation of the Poisson distribution.

We use the case $\gamma = 0$ of the generalized phase retrieval algorithms, which is given by

$$\rho_{n+1}(\boldsymbol{r}) = \rho_n(\boldsymbol{r}) \exp\{\lambda(\rho_n(\boldsymbol{r})' - \rho_n(\boldsymbol{r}))\}, \tag{24}$$

because D_γ with $\gamma = 0$ is equal to the Kullback-Leiber divergence and its minimization corresponds to the maximum entropy method. As the parameter in Eq. (24), λ needs to be sufficiently small, because $\rho(\boldsymbol{r})$ diverges to infinity in the process of computer simulation. However, many iterations are required to obtain a plausible object using a sufficient small λ. Then, we use the scheduled parameter depending on the number of iterations n, $\lambda(n) = \epsilon(1 - \frac{n}{1+M})$, where ϵ is a positive constant and M is the maximum number of iterations.

The target object ρ_{target}, which is shown in Fig. 5 (a), is a two-pillars object on the one-dimensional discrete object domain (the size is 256). The random objects are used as the initial start for the algorithms, In the first process, 500 iterated HIO is used and the weakly estimated object is obtained. And then, in the second process, $\gamma = 1$ (1500 iterations) and $\gamma = 0$ (1500 iterations) are compared using the estimated object as the initial start. The case of $\gamma = 1$ ($\lambda = 1$) is related to the ER algorithm. The case of $\gamma = 0$ is related to an iterative MEM phase retrieval algorithm. The Fourier-domain constraint is given by the Fourier intensity of Fig. 5 (a) with the contamination of the Poisson noise given by Eq. (23). The object support is used as the object-domain constraint. That is, the value of the target object is zero on the object domain expect for the the support. Figures 5 (b) and (c) are the obtained objects by using $\gamma = 1$ and $\gamma = 0$, respectively. Figure 5 (d) shows the obtained objects by the two methods for comparing them. Three typical differences between them are presented in the right side of the figure. In each case, a coarse image of the target object is reconstructed. However, great influence of the noise is found in the case of $\gamma = 1$, and such the influence in the case of $\gamma = 0$ is smaller than that of $\gamma = 1$. As a result, the algorithm of $\gamma = 0$ has an efficiency in the case of the Fourier intensity contaminated by Poisson noise.

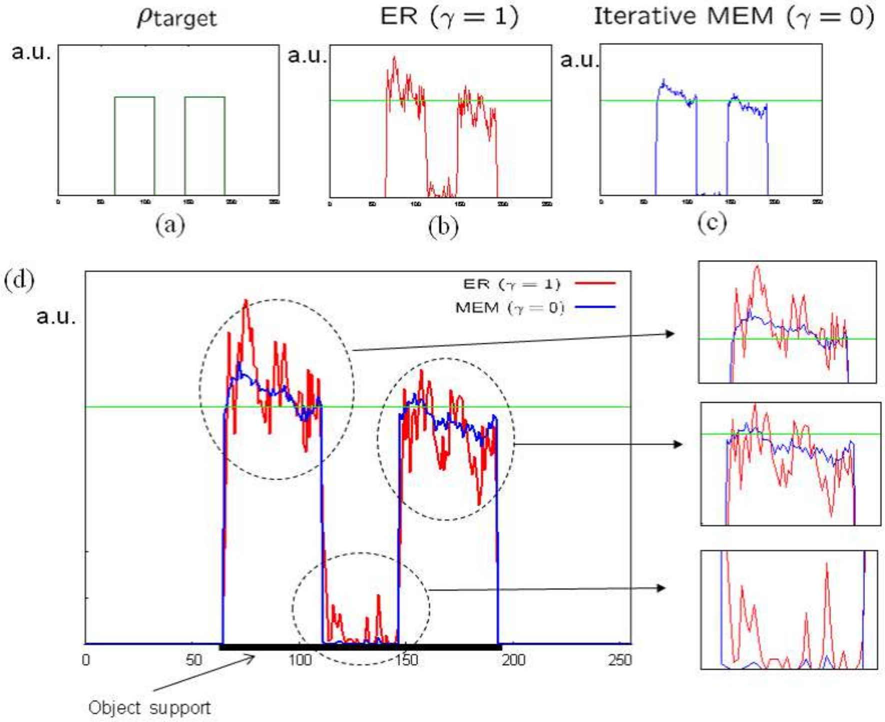

Figure 5: (a) The target object, (b) the object obtained by ER ($\gamma = 1$), (c) the object obtained by the iterative MEM algorithm ($\gamma = 0$), (d) The obtained objects by the two methods are presented. The typical differences between them are presented in the right side of the figure.

5. Conclusion

The phase retrieval has been widely treated in measuring the diffraction waves. In the progress of the diffractive imaging for non-periodic objects, various advanced experimental results have been presented. In this paper, based on the generalized phase retrieval algorithms presented in [17], we introduce an information-theoretic approach to phase retrieval. And also, we newly show a refined derivation of the algorithms with an example of the algorithms using the Poisson-noise-contaminated Fourier intensity.

The analysis for phase retrieval is important for obtaining the certain results from the experimental diffraction patterns. Recently, some experimental results using an advanced electron microscope was presented by our research group [6, 7, 8], and we presented the advanced theoretical and computational results [19, 20]. Hereafter, an information-theoretic analysis of phase retrieval using various kinds of incomplete Fourier intensities are one of our future works.

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