Phase Scatterer Optimization for Phase Retrieval in Coherent Diffraction Imaging

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In coherent diffractive imaging (CDI), the well-known non-convex formulation of the phase retrieval problem, the task is to recover a complex-valued object $\mathbf{x} \in \mathbf{C^N}$ from the magnitude of its Fourier transform $\mathbf{b}$. To do this, the equation is solved

$$\mathbf{b} = |\mathbf{Fx}| + \omega \tag{1}$$

where $\mathbf{F}$ is the Fourier transform operator and ω is a noise. To recover $\mathbf{x}$ from $\mathbf{b}$ they usually use a least-squares cost (which coincides with the maximum likelihood criterion, assuming Gaussian noise)

$$\underset{x \in C^N}{\textbf{minimize}} \; \|\mathbf{b} - |\mathbf{Fx}|\|^2 \tag{2}$$

Note that in the presented work we used equation (1) not only for case Fraunhofer diffraction but also for Fresnel one, and estimate (2) not only for Gaussian, but also other types of noise, Poisson, Exponential and so on. The justification for such a not entirely strict expansion of the problem statement was the successful calculations we performed.

A number algorithms of alternate projection (AP-algorithms) for solving problem (1, 2) are known, the success of which depends significantly on the method of their initialization [1–4]. One of the most popular ways to initialize these algorithms is to use a random phase scatterer in the spectral plane. In this paper, we show how the performance of both our AP algorithm using amplitude binary masks (APBM) [1] and other known AP algorithms can be improved by using the characteristics of random phase scatterers in their entirety, which has not been done before.

1. Degrees of freedom of phase scatterers

The use of a scatterer $\mu(t) = e^{i\varphi(t)}$, where $\varphi(t)$ is a uniform distribution of random phase in the interval $\varphi(t) \in (0, 2\pi)$, to initialize the AP-algorithm was first proposed by Gerchberg and Saxton in 1972 [2] when solving the D1 version of the phase problem. This usage has become standard in a certain sense, sometimes in works on phase problem D1 or D2 its type and phase range are assumed by default. Later, having noticed the dependence of the accuracy of the solution to the problem on a specific instance of $\mu(t)$, they began to use enumeration (generation) of various instances of uniform $\mu(t)$ in order to select the best of them.

Now let us consider the problem of using a phase scatterer to initialize AP algorithms in a more general setting. Let us introduce the concept of a random phase scatterer D2 of a general type, which we denote by $\varphi(\mathbf{r})$, $\mathbf{r} = (x, y)$. Obviously, the number of degrees of freedom of the random distribution $\varphi(\mathbf{r})$ when using it as a free parameter of the AP algorithm is not less than three. That is, we can control:

$$\left.\begin{array}{l} a - \textit{type} \text{ of random distribution of } \varphi(\mathbf{r}) \text{ (Uniform, Normal, Poisson and so on);} \\ b - \text{a particular } \textit{sample } \varphi(\mathbf{r}) \text{ of a given distribution type;} \\ c - \text{the } \textit{interval } \Delta\varphi \text{ of random phases in this particular sample } (0 < \varphi(\mathbf{r}) < \Delta\varphi). \end{array}\right\} \tag{3}$$

Note that of the three degrees of freedom listed for $\varphi(\mathbf{r})$, only (a), (b) and only for the Uniform distribution are used in known works on the phase problem, while (c) is not used at all. However, as our calculations show, by controlling all three degrees of freedom of the phase scatterer, it is possible to significantly accelerate the convergence of algorithms and increase the accuracy of the obtained solutions.

Below are the results of model experiments with APBM, as well as with well-known algorithms [4].

2. Numerical Simulations

2.1. We first illustrate the effectiveness of phase scatterer control (3) using an example taken from the classic work of Gerchberg-Saxton [2]. The authors explain the stagnation of their GS algorithm in the example with the object function $f(t) = \text{rect}(2t) \cdot \exp\left(i \cdot 30\pi t^2\right)$ and the modulus of its Fourier spectrum (see Fig. 3 and detailed of squared error history in Table 1 [2]) by inadequate sampling in either of the two domains, despite the fact that the sampling increment $\Delta t = 1/128$, with a total number of samples N = 256, satisfies the Shannon-Wittaker theorem. As already noted, the authors used the scatterer $\mu(t) = e^{i\varphi(t)}$ with an unchangeable, during the calculation, uniform phase distribution $\varphi(t) \in (0, 2\pi)$.

It is easy to show how, leaving the sampling increment Δt and the number of samples N unchanged, by optimizing $\varphi(t)$ one can obtain a set of local solutions to the problem. In this case, it was sufficient to use only one (3c) degree of freedom of the existing uniform random phase distribution $\varphi(t)$. For this, the phase interval $\varphi(t)$ is represented in the form $(0,\ k\Delta)$, where $k = 1, 2, \ldots$, and $\Delta = c_0\pi$ is the step along the phase interval ($c_0 < 1$ is a constant determining the step size). By setting c_0 and running the GS algorithm for each $(0,\ k\Delta)$ phase interval, we find the phase intervals of the scatterer in which the phase of the Fourier spectrum of the function $f(t)$ is reconstructed with an accuracy up to a constant phase (Fig. 1). As expected, for the $(0, 2\pi)$ phase interval of the scatterer (dash-dotted line at $k = 20$), as in [2], the solution does not exist. Note that in the 2D version of the given example, to find the set of local solutions, it is sufficient to walk with the same step over the range $(0, 2\pi)$.

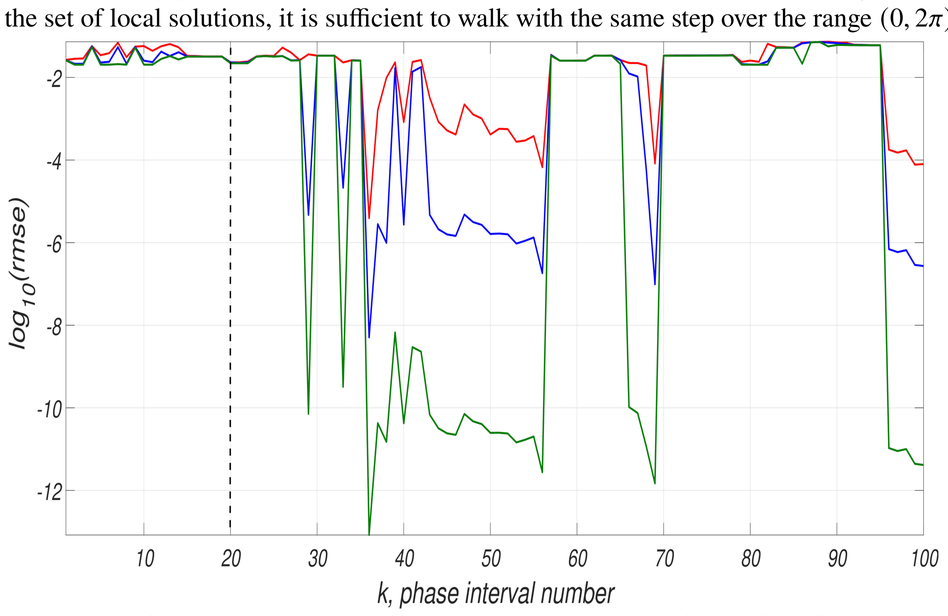

Fig. 1: Semi-log plot of the reconstruction error vs the phase interval number k of the uniform distribution $\varphi(t)$ of the computational illumination $\mu(t) = e^{i\varphi(t)}$. Phase step $\Delta = c_0\pi$, $c_0 = 0.1$. Value $k = 20$ corresponds to the $(0, 2\pi)$ phase interval (marked by the dashed line). Number of GS iterations: red – 50, blue – 100, green – 200.

2.2. Taking into account the advanced capabilities of phase scatterers for initializing AP algorithms described in Section , we performed model experiments to solve the CDI problem for a number of complex-valued objects. Some of the obtained results are presented in Fig. 2–4. Algorithms APBM and ER, HIO, and RAAR [1,3,4] were used. The Uniform, Normal, Exponential, Poisson, LogNormal, Gamma, Beta, and Binomial distributions for phase scatterers generated with Matlab were used. The distribution parameters were set arbitrarily during their generation.

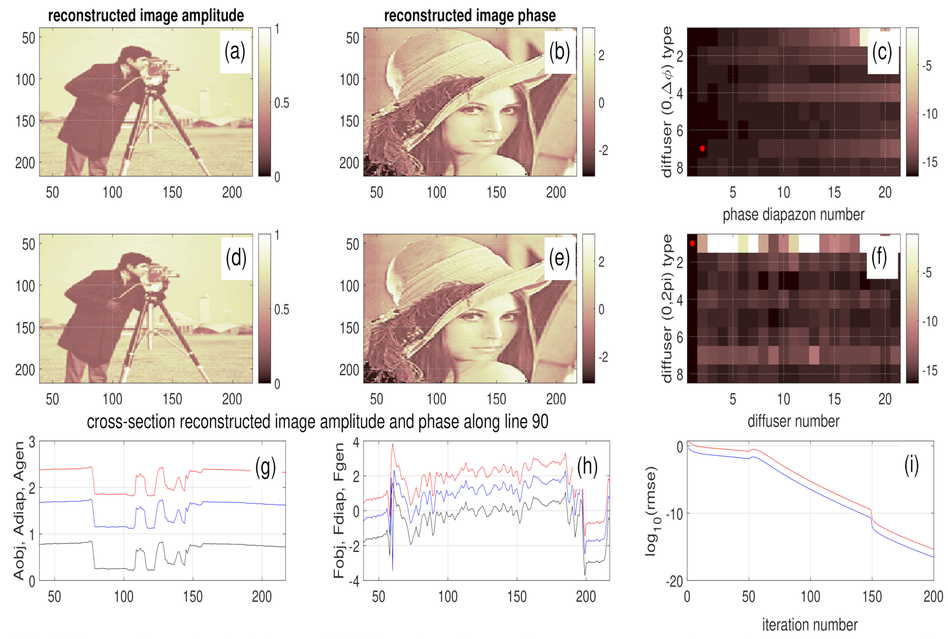

Fig. 2: 256x256 complex-valued objects. APBM – algorithm with support constraint and oversampling equal to 2: a, d – amplitude, b, e – phase of reconstructed object by the method of 1) enumeration of phase ranges or 2) enumeration of $(0, 2\pi)$-instances of scatterer, respectively, for 8 types of scatterers, Red mark in (c), (f) indicates the optimal type and phase range or type and $(0, 2\pi)$-instance of scatterer, selected for calculation; g, h – cross-sections of reconstructed amplitudes and phases, respectively, where black – ideal, dlue – method 1, red – method 2; i – algorithm convergence graph for both methods.

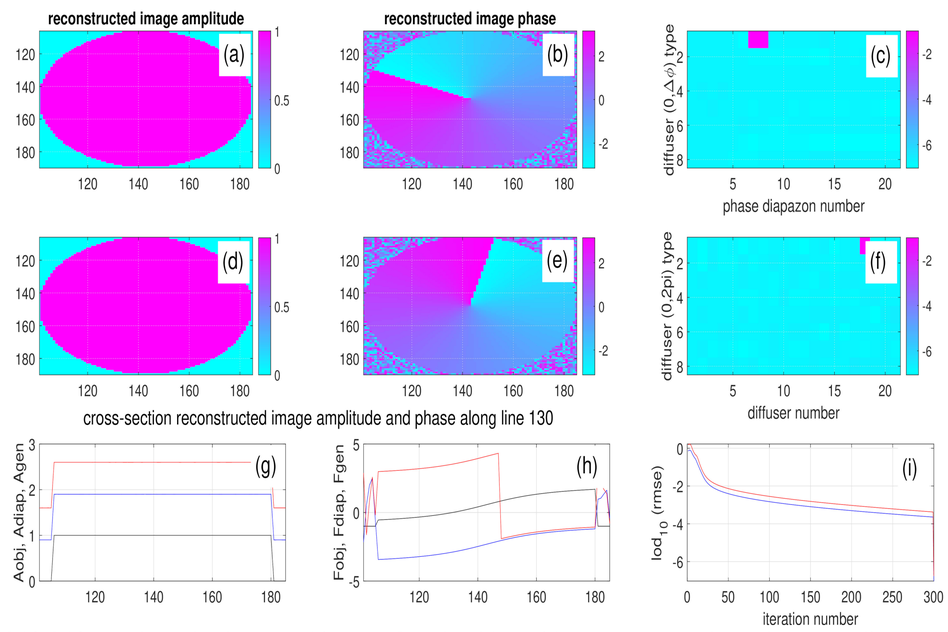

Fig. 3: 256x256 complex valued vortex object. HIO – algorithm with support constraint and oversampling equal to 3: a, d – amplitude, b, e – phase of reconstructed object by the method of 1) enumeration of phase ranges or 2) enumeration of $(0, 2\pi)$-instances of scatterer, respectively, for 8 types of scatterers, Red mark in (c), (f) indicates the optimal type and phase range or type and $(0, 2\pi)$-instance of scatterer, selected for calculation; g, h – cross-sections of reconstructed amplitudes and phases, respectively, where black – ideal, blue – method 1, red – method 2; i – algorithm convergence graph for both methods.

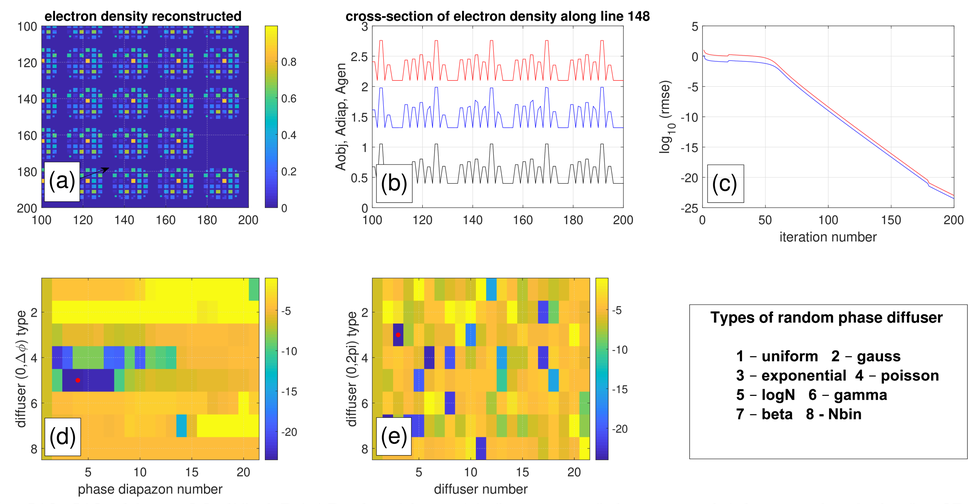

Fig. 4: 512x512 object. Modified RAAR algorithm: (a) fragment of the restored 'electron density' of a 2D crystal reconstructed from the known modulus of its Fourier spectrum. The crystal was modeled on a 512x512 pixel grid with an oversampling ratio $\sigma = 2.41$ and consisted of 15x15 cells. The density of the unit cell with a size of 22x22 pixels and 6x6 randomly distributed 'atoms'; (b) cross-sections (a) along line 148, where black – ideal, dlue – method 1, red – method 2 reconstruction; (c) convergence graph of the algorithm, (d), (e) indicates the optimal type and phase range or type and $(0, 2\pi)$-instance of scatterer, selected for calculation.

3. Conclusion

The article shows how to improve the efficiency of AP algorithms for solving the CDI problem using the degrees of freedom of random phase scatterers that have not been used so far. Note that properties (a) and (c) of the scatterers in (3) can compete with each other in the accuracy of the solution and the convergence rate of the iterative algorithm depending on the type of the object under study. At the same time, the advantage of property 3(c) is that there is no need to generate new instances of a scatterer of a given type at each iteration step; it is sufficient to increase the phase range of a single scatterer of a given type, starting from the it's minimum range.

References

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