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New method for probe position correction for Ptychography

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ABSTRACT

For high resolution imaging, X-rays and electron beams are being used. However, for such a short wavelength, imaging with lenses becomes difficult as lenses absorb a part of radiation and lenses with very low aberrations must be used. Ptychography is a lens-less imaging technique which uses intensity information of the multiple diffraction patterns in the far field. These multiple far field diffraction patterns are generated by an unknown object which is scanned by a localized illuminated spot (probe).

Accurate knowledge of initial parameters is important for a good reconstruction of the object. Robustness of the Ptychography Iterative Engine (PIE) has already been studied for inaccurately known initial parameters, where the success of the algorithm was found to be sensitive to the accuracy of the estimate of lateral positions of the probe.

We present here a new method to correct the lateral position of the probe with respect to the object. This method is more straightforward to implement than other existing algorithms while comparable accuracy for the lateral position is achieved. Being able to correct the probe positions has positive implication in experiments, in particular at the short wavelength cases. It relaxes the requirement for the experimental set-up.

Keywords: Phase retrieval, Ptychography, Image reconstruction technique

1. INTRODUCTION

Short wavelength e.g: X-rays, electron beams are being used for high-resolution imaging, but the requirement for lenses are usually very high and the experiments can be very complex. Hence, lens-less imaging was introduced. In lens-less imaging, diffraction patterns of an object are captured in the far field. Since cameras can only detect the intensity pattern, the phase information is lost during this process. There are many existing iterative algorithms which can solve the phase problem. The most used ones are Error Reduction (ER) algorithm[1] and the Hybrid Input-Output (HIO) algorithm.[2]

Coherent Diffractive Imaging (CDI) is a type of lens-less imaging. In CDI, the intensity of the far-field of an illuminated object is used to reconstruct an object. Ptychography[3,4] is a form of CDI where the object is illuminated and scanned by a localized probe or aperture in a way that the probe at neighbouring scan positions overlaps, and these recorded multiple far-field intensity patterns corresponding to the different probe positions are used to reconstruct the object. The redundant information due to the overlap between neighbouring probes is an important aspect for the fast convergence and successful reconstruction of the object. The optimum overlap between neighbouring probe positions is found to be 60%.[6] However, this optimum overlap depends on the type of object, probe, and the size of probe. The algorithm that is used for the reconstruction, is called Ptychographical Iterative Engine (PIE).[5] In Fig 1, the object is scanned by a probe in a 8 × 8 grid configuration.

A few variants of PIE have been developed, for example, ePIE[7] is an extension of PIE which can reconstruct the object as well as the localized probe function. This is useful when the accurate knowledge of probe is difficult to obtain. Ref. by Thibault at al.[8] to retrieve probe also perform well, however the noise level should be low and a fair guess of probe should be known. fPIE[9] can reconstruct the object even though the measured intensity patterns are under sampled, and in a recent study,[10] the PIE and its variants have been improved with the combination of the Hybrid Input-Output algorithm.[2]

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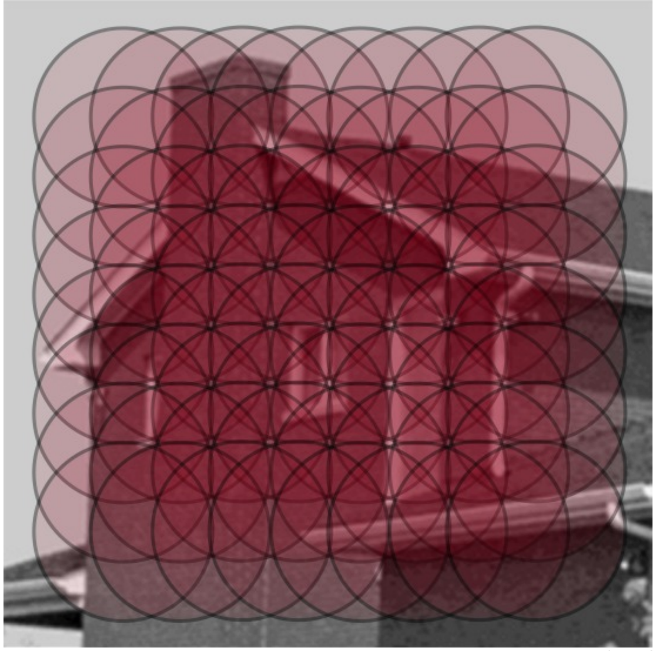

Figure 1: Object is scanned by a probe. Intensity patterns are recorded in the far field. In PIE, these intensity patterns are used to reconstruct the object.

We have used ePIE in our simulations for reconstructing the object as well as the probe function. This algorithm is found to be sensitive for errors in the estimated transverse positions of the probe function which limit the reconstruction of the object and the probe function, in particular when imaging with X-rays or electron beams,[11,12] for example, 50 pm of accuracy in the probe positions is required for electron ptychography.[19] This amount of accuracy is difficult to achieve as even the thermal shift could lead to the degraded reconstruction in electron ptychography.

Some advances have already been made to relax the extreme accuracy in the knowledge of the probe positions. Some probe position correction methods were explored.[15,16] These methods require human intervention and are computationally expensive. If the model of positioning error is known, one can use a method developed by Beckers at al.,[18] whereas the "annealing approach"[17] uses the trial and error method. A recent developed technique based on finding the cross correlation of two consecutive object estimates for each probe position is found to be successful for correcting the probe position with sub-pixel accuracy.[19] However, to find the probe positions with sub-pixel accuracy, the authors use an additional method for sub-pixel registration.[20]

A nonlinear (NL) optimization approach[14] was proposed to correct the probe positions; however, the position correction is shown when the error in initial probe positions is less than one pixel. In this work, NL optimization approach is being used to update the object, probe and the probe positions which could easily lead to local minima. The NL optimization was improved in the conjugate gradient (CG) method[21] to correct probe positions by using CG method only to update the probe positions whereas ePIE and difference map are being used for object and probe update. However, the CG method can retrieve the probe positions only to pixel accuracy.

In this work, we propose a novel method to correct probe positions.

2. THE ALGORITHM

In ptychography, an object is scanned by an illuminating probe, and for each probe position the far field intensity pattern is recorded. If the object transmission function and the probe function shifted to probe position $\mathbf{R_j}$ are denoted as $O(\mathbf{r})$ and $P(\mathbf{r}-\mathbf{R}_j)$ respectively. The exit wave function can be written as

$$\psi^j(\mathbf{r}) = O(\mathbf{r})P(\mathbf{r}-\mathbf{R}_j), \tag{1}$$

where $\mathbf{r} = (x, y)$ is a coordinate vector in the object plane and the probe is shifted by a vector $\mathbf{R}_j = (X_j, Y_j)$. $\mathbf{R}_j$ is chosen such that probes at neighbouring scan positions overlap with each other.

The measured intensity pattern of the far field plane can be written as

$$I^j(\mathbf{u}) = |\mathscr{F}\{\psi^j(\mathbf{r})\}|^2, \tag{2}$$

where $\mathbf{u}$ is a coordinate vector in the far field plane and $\mathscr{F}$ denote the Fourier transform. Here we follow the same steps as ePIE[7] where the object and the probe function updates are performed in series. The algorithm starts with initial guessed object and probe function which are denoted as $O_g(\mathbf{r})$ and $P_g(\mathbf{r})$ respectively. The steps for the k^{th} iteration are as follows

1. Start with a guessed object function $O_k(\mathbf{r})$ and a guessed probe function $P_k(\mathbf{r})$.
2. Using equation 1, calculate the estimated exit wave function for the probe position $\mathbf{R}_j$.
$$\psi_k^j(\mathbf{r}) = O_k(\mathbf{r})P_k(\mathbf{r} - \mathbf{R}_j) \tag{3}$$
3. Propagate the field $\psi_k^j(\mathbf{r})$ to the far field plane, in other words, apply the Fourier transform to $\psi_k^j(\mathbf{r})$.
$$\Psi_k^j(\mathbf{u}) = \mathscr{F}\{O_k(\mathbf{r})P_k(\mathbf{r} - \mathbf{R}_j)\} \tag{4}$$
4. Apply the amplitude constraint by replacing the amplitude of guessed diffraction pattern with the known amplitude of the measured intensity.
$$\Psi_k'^j(\mathbf{u}) = \sqrt{I^j(\mathbf{u})}\frac{\Psi_k^j(\mathbf{u})}{|\Psi_k^j(\mathbf{u})|} \tag{5}$$
5. Back propagate the field $\Psi_k'^j(\mathbf{u})$ to the object plane, by applying the inverse fourier transform to $\Psi_k'^j(\mathbf{u})$.
$$\psi_k'^j(\mathbf{r}) = \mathscr{F}^{-1}\{\Psi_k'^j(\mathbf{u})\} \tag{6}$$
6. Update the object function using the following update equations.
$$O_{k+1}(\mathbf{r}) = O_k(\mathbf{r}) + \frac{P_k^*(\mathbf{r} - \mathbf{R}_j)}{|P_k(\mathbf{r} - \mathbf{R}_j)|^2_{\max}}\alpha_1(\psi_k'^j(\mathbf{r}) - \psi_k^j(\mathbf{r})) \tag{7}$$
where we choose the parameter α_1 to be 1.
7. Update the probe function using the new updated object function as follows
$$P_{k+1}(\mathbf{r}) = P_k(\mathbf{r}) + \frac{O_k^*(\mathbf{r} + \mathbf{R}_j)}{|O_k(\mathbf{r} + \mathbf{R}_j)|^2_{\max}}\alpha_2(\psi_k'^j(\mathbf{r}) - \psi_k^j(\mathbf{r})) \tag{8}$$
where the parameter α_2 is also chosen to be equal to 1.

   To correct the probe positions, we use the difference in the estimated intensity and the measured intensity patterns in the far field for each probe positions. Then, we decompose this difference ΔI^j in terms of error $(\Delta X_j, \Delta Y_j)$ in the probe position (X_j, Y_j).
$$\Delta I^j \approx \frac{\partial I^j}{\partial X_j}\Delta X_j + \frac{\partial I^j}{\partial Y_j}\Delta Y_j. \tag{9}$$
   So the update equation for the probe position (X_j, Y_j) will become as
$$X_{j,k+1} = X_{j,k} - \beta\Delta X_j, \tag{10}$$
$$Y_{j,k+1} = Y_{j,k} - \beta\Delta Y_j, \tag{11}$$
   Here, β is a feedback parameter which defines the step size of update in the probe positions.

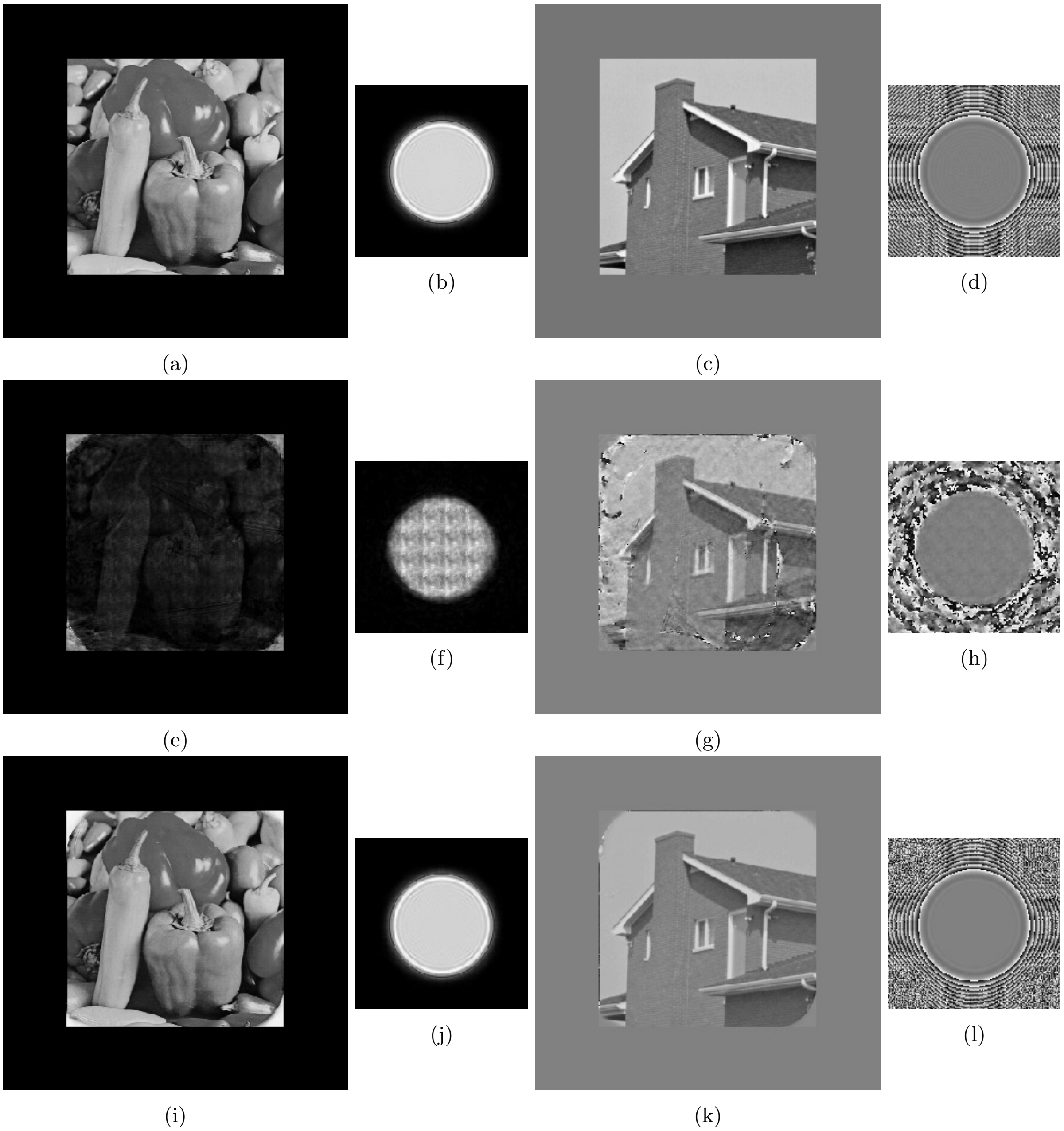

Figure 2: Comparison of the reconstructed object amplitude and phase with and without position correction. The object is scanned by a 8×8 probe positions with an overlap of 78%. Here, a random error of $10\Delta x$ in the probe positions was added. (a) and (c) are the test object amplitude varying from $[0, 1]$ and the object phase varying from $[-0.7\pi, 0.7\pi]$. (b) and (d) are the probe amplitude and the probe phase respectively. (e) and (g) are the amplitude and phase of the reconstructed object without position correction. (i) and (k) are the amplitude and phase of the reconstructed object using position correction refinement.

3. SIMULATIONS

The robustness of the algorithm was analysed using the simulated data. Here, the parameters are chosen in such a way that the set-up represents a visible light experiment. The probe was formed by a Fresnel propagation of light through a pinhole of diameter 700 μm, where the wavelength of light was 500 nm. The propagation distance from the pinhole was 1 mm. The diffraction patterns were created using a test object shown in Fig. 2(a) and

2(c). The object has 256×256 pixels. The object amplitude was created using 'Peppers' and the magnitude varied between $[0, 1]$. The object phase was created using 'House' and the phase varied between $[0.7\pi, 0.7\pi]$. A regular grid of 8×8 was formed with an interval of 171.4 μm. Then a random offset of $[10, 10]$ pixels or [78, 78] μm was added to each intersection. The resulted intersection were used for the probe positions and to generate the diffraction pattern in the far field.

Figs. 1(a-d) show the test object and the probe. Figs. 1(e-h) show the reconstruction of the object and the probe without the probe position correction. Figs. 1(i-l) show the reconstruction of the object and the probe with position correction.

4. CONCLUSION AND OUTLOOK

Here we have proposed a new method to correct the probe positions in Ptychography. The difference between measured intensity and estimated intensity is used. More quantitative analysis of this method such as its robustness in presence of noise and experimental validation will be the subject of further investigation.

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