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Ptychographic phase retrieval by applying hybrid input-output (HIO) iterations sequentially

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ABSTRACT

We have designed a ptychographical algorithm (HIO-PIE) in which HIO (Hybrid Input-Output) iterations are applied for each probe position sequentially. Simulations indicated that HIO-PIE tends to outperform PIE (Ptychographical Iterative Engine) even in the presence of shot noise, especially when the number of probe positions is small. Thus, this adaptation may reduce the number of scan positions required for a successful image reconstruction, thereby relaxing the constraints on an experimental setup. In this article, experimental results obtained using an SLM (spatial light modulator) and visible laser light (633 nm) show that when few probe positions are used, HIO-PIE converges significantly faster than PIE.

Keywords: Ptychography, Coherent Diffractive Imaging, Phase retrieval

1. INTRODUCTION

Coherent diffractive imaging (CDI) is a technique that can be used to image a sample without having to use lenses. Especially for X-ray imaging this may be useful, since the reconstructed image will not suffer due to low-quality focusing optics. However, because one cannot measure complex-valued fields directly but only the intensity, one needs to retrieve the phase of the diffracted field in order to reconstruct the amplitude. Algorithms that deal with the phase retrieval problem have been developed since the 1970's. Gerchberg and Saxton introduced in 1972 an algorithm with which the phase of a field can be reconstructed if the intensity is known in two planes perpendicular to the direction of propagation.¹ The algorithm works straightforwardly by propagating the field back and forth between the two planes, each time setting the calculated amplitude equal to the measured amplitude (i.e. applying the amplitude constraint) while keeping the calculated phase. In 1978, Fienup modified the Gerchberg-Saxton algorithm to fit a different set of constraints.² Instead of having two intensity measurements, this algorithm uses a support constraint in one plane (meaning that the object has finite known size), and an amplitude constraint in the other plane. This algorithm is referred to as the Error Reduction (ER) algorithm, and Fienup demonstrated in 1982 that it can be interpreted as using the steepest-descent method to minimize a sum-of-squares cost functional.³ Another algorithm that Fienup introduced to improve convergence is the Hybrid Input-Output (HIO) algorithm. The difference between HIO and ER is that HIO uses a feedback function outside the object's support. In 2002, Bauschke et al. identified the HIO algorithm as a nonconvex Douglas-Rachford algorithm.⁴ Based on this observation, other projection-based phase retrieval algorithms have been developed such as the Relaxed Averaged Alternating Reflections (RAAR) algorithm.⁵

In 2004 Faulkner and Rodenburg introduced another CDI method named ptychography.⁶ In ptychography, the object is illuminated with a probe that is shifted to different probe positions, such that the probes at neighbouring positions overlap with each other. For each probe position a far-field intensity pattern is recorded, and with this set of diffraction patterns the object is reconstructed using an algorithm called the Ptychographic Iterative Engine (PIE). Due to the overlap between probes, there is redundant information present in the recorded diffraction patterns, that makes a ptychographic reconstruction more robust than the ER algorithm. In fact, if we assume that the probe has a finite support, the PIE algorithm can be interpreted as applying ER iterations

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to each probe position sequentially. Given that ER had been demonstrated to be an instance of the steepest-descent method applied to a cost function minimization problem, and given the close relation between PIE and ER, it should not come as a surprise that in 2008 Guizar-Sicairos and Fienup demonstrated PIE was also closely related to the minimization of a cost functional using a steepest-descent method.⁷ The main difference between the PIE algorithm and the steepest-descent algorithm is that PIE updates in each iteration the object for each probe position sequentially, while in the steepest-descent algorithm the object is updated in its entirety each iteration. In 2016 Zuo et al. termed these methods the ‘incremental gradient’ and ‘global gradient’ solutions respectively,⁸ and they remarked that the global methods are less cost efficient and converge more slowly than the incremental method, though the incremental method seems to be more susceptible to noise. Since there are more sophisticated optimization methods than the steepest-descent method and the ER algorithm, naturally it has been explored to tackle ptychography with more advanced methods such as the conjugate-gradient method, the Gauss-Newton method, or HIO, as has been done by Qian et al. in 2014.⁹ However, this study was limited to global methods. In 2016, we explored the possibility to combine PIE with HIO as an incremental method by introducing a feedback function per probe position.¹⁰ Simulations indicated that HIO-PIE requires fewer probe positions to obtain a good object reconstruction, and that in general it converges faster than PIE. By updating the amplitude constraint it was shown that HIO-PIE could be made more robust against noise, and the effect of updating the amplitude constraints on noise-robustness has been considered further.¹¹

In this article we test HIO-PIE in a proof-of-principle experiment using visible light and Spatial Light Modulator (SLM) to create and scan the object.

2. THEORY

In this section we briefly describe PIE and the proposed HIO-PIE algorithm which we will compare. In sequential HIO-PIE, as we proposed in,¹⁰ we update the guessed object one probe position at a time, but at the same time we have a feedback function $B(\mathbf{r})$ (as in HIO) per probe position to improve the convergence.

Sequential/incremental PIE:

1. We start with the n^{th} guessed object $O_{g,n}(\mathbf{r})$.
2. For a certain probe position \mathbf{R} we calculate the guessed exit wave $\psi_{g,n}(\mathbf{r}, \mathbf{R}) = O_{g,n}(\mathbf{r})P(\mathbf{r} - \mathbf{R})$.
3. We calculate the guessed diffracted field $\Psi_{g,n}(\mathbf{k}, \mathbf{R}) = \mathcal{F}\{\psi_{g,n}(\mathbf{r}, \mathbf{R})\}$.
4. We replace the amplitude of the guessed diffracted field $\Psi_{g,n}(\mathbf{k}, \mathbf{R})$ with the measured amplitude of the diffracted field $\Psi(\mathbf{k}, \mathbf{R})$, while keeping the phase of $\Psi_{g,n}(\mathbf{k}, \mathbf{R})$. This gives the corrected guessed diffracted field $\Psi_{c,n}(\mathbf{k}, \mathbf{R}) = \frac{\Psi_{g,n}(\mathbf{k}, \mathbf{R})}{|\Psi_{g,n}(\mathbf{k}, \mathbf{R})|} |\Psi(\mathbf{k}, \mathbf{R})|$.
5. We obtain a corrected guess for the exit wave function by inverse Fourier transforming the corrected guess of the diffracted field $\psi_{c,n}(\mathbf{r}, \mathbf{R}) = \mathcal{F}^{-1}\{\Psi_{c,n}(\mathbf{k}, \mathbf{R})\}$.
6. We update the guess of the object in the region where the probe $P(\mathbf{r} - \mathbf{R})$ is sufficiently strong:

$$O_{g,n}(\mathbf{r}) := \begin{cases} \psi_{c,n}(\mathbf{r}, \mathbf{R}) \frac{P^*(\mathbf{r} - \mathbf{R})}{\max |P(\mathbf{r} - \mathbf{R})|^2} & \text{if } |P(\mathbf{r} - \mathbf{R})| \geq \alpha, \\ O_{g,n}(\mathbf{r}) & \text{if } |P(\mathbf{r} - \mathbf{R})| < \alpha. \end{cases} \quad (1)$$

Here, α is a small parameter to prevent errors from blowing up such where $|P(\mathbf{r} - \mathbf{R})|$ is small. α should be chosen sufficiently small so the entire object is covered by the update regions. Once we have done this for all probe positions \mathbf{R} , one iteration is completed and we can set $O_{g,n+1}(\mathbf{r}) = O_{g,n}(\mathbf{r})$.

Sequential/incremental HIO-PIE:

1. We start with the n^{th} guessed object $O_{g,n}(\mathbf{r})$, and the n^{th} feedback function $B_n(\mathbf{r}, \mathbf{R})$ for probe position \mathbf{R} . The initial value of the feedback function is $B_0(\mathbf{r}, \mathbf{R}) = 0$.

2. For a certain probe position \mathbf{R} we calculate the guessed exit wave $\psi_{g,n}(\mathbf{r}, \mathbf{R}) = O_{g,n}(\mathbf{r})P(\mathbf{r} - \mathbf{R})$.
3. We calculate the guessed diffracted field $\Psi_{g,n}(\mathbf{k}, \mathbf{R}) = \mathcal{F}\{\psi_{g,n}(\mathbf{r}, \mathbf{R}) + B_n(\mathbf{r}, \mathbf{R})\}$.
4. We obtain a corrected guess for the exit wave function $\psi_{c,n}(\mathbf{r}, \mathbf{R})$ as in steps 4-5 of Sequential PIE.
5. We update the feedback function in the region where the probe is sufficiently weak:

$$B_{n+1}(\mathbf{r}, \mathbf{R}) = \begin{cases} 0 & \text{if } |P(\mathbf{r} - \mathbf{R})| \geq \alpha, \\ B_n(\mathbf{r}, \mathbf{R}) - \beta\psi_{c,n}(\mathbf{r}, \mathbf{R}) & \text{if } |P(\mathbf{r} - \mathbf{R})| < \alpha. \end{cases} \quad (2)$$

β is the HIO feedback parameter which we choose to be 0.9.

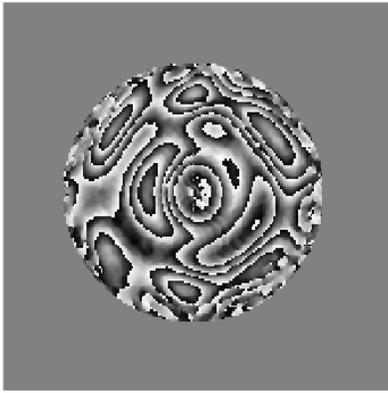
6. We update the guess of the object as in Sequential PIE according to Eq. (1).

3. METHOD

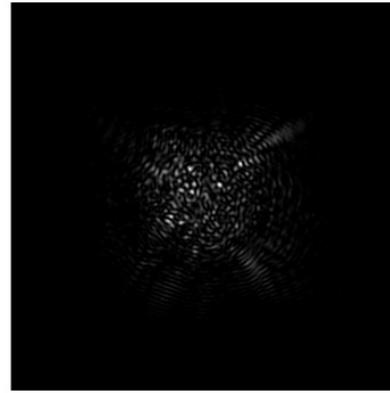
To obtain an experimental ptychographical dataset to test the proposed algorithm on, we use a phase-only Spatial Light Modulator (Holoeye Pluto SLM, 1920×1080 pixels, $8.0 \mu\text{m}$ pixel pitch) that is illuminated by a collimated laser beam (HeNe laser, wavelength of 633nm). By assigning a pattern to the SLM we create a phase object, and by shifting the assigned pattern we can shift the object as is required for ptychography. We use a lens (focal length 15cm) to create the Fourier transform of the field reflected by the SLM, though in an X-ray experiment the Fourier transform would be created by far-field propagation. In CDI, the resolution with which an object can be reconstructed depends on how high spatial frequencies can be captured, which depends on the Numerical Aperture (NA) of the detector, but also on the noise level and the dynamic range of the diffraction pattern. It has been pointed out that for both X-ray experiments¹² and visible light experiments¹³ it is beneficial to use illumination with a wild phase pattern so that the dynamic range of the diffraction patterns are reduced, which means less information is lost due to detector noise. In our experiment, we can achieve this by assigning a fixed wild phase pattern on top of the shifting object with the SLM.



(a) Phase object



(b) Phase of the probe

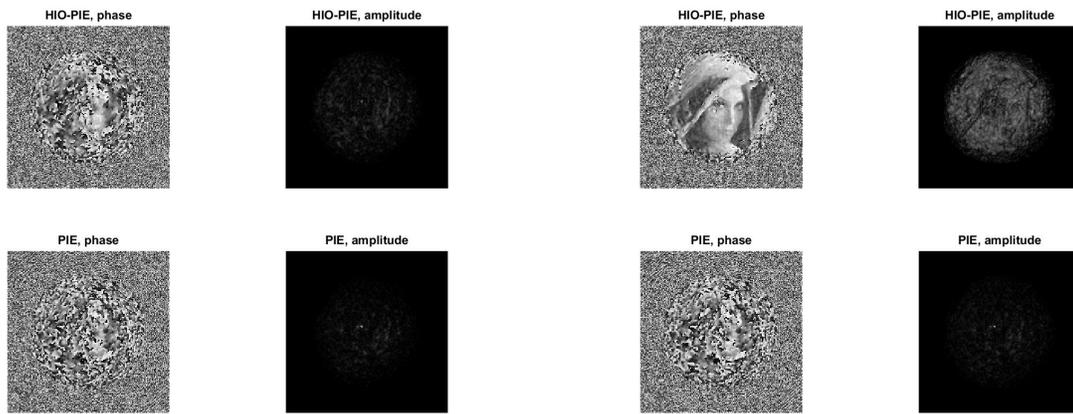


(c) Recorded diffraction pattern

Figure 1: (a) ‘Lena’ image that is assigned to the SLM to serve as a phase object. The phase ranges from 0 to $0.9 \times 2\pi$. (b) Wild phase pattern assigned to the SLM to reduce the dynamic range of the diffraction patterns. (c) One of the recorded diffraction patterns.

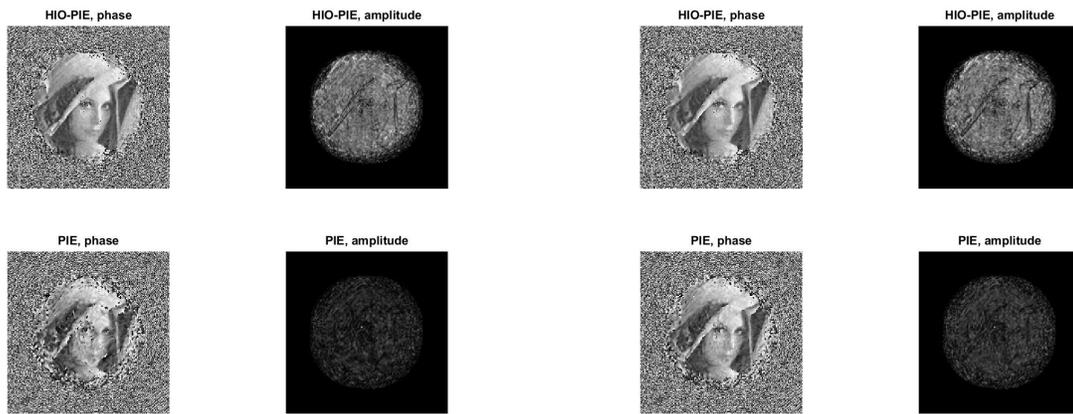
4. RESULTS

The results shown in Fig. 2 demonstrate that for 2×2 probe positions, HIO-PIE gives an object reconstruction significantly faster than PIE: HIO-PIE takes around 15 iterations, while PIE takes around 45 iterations. However, the more probe positions are used, the smaller the difference in convergence rate becomes. It is shown in Fig. 3 that when 3×3 probe positions are used, HIO-PIE gives a decent result after 4 iterations, while PIE takes around 7 iterations. However, it is important to keep in mind that even though the difference in the required number of iterations has become smaller by increasing the number of probe positions, each iteration has become more computationally expensive when more probe positions are involved. When 4 probe positions are used, HIO-PIE saves $4 \cdot (45 - 15) = 120$ object updates, and when 9 probe positions are used, HIO-PIE saves $9 \cdot (7 - 4) = 27$ object updates.



(a) 10 iterations

(b) 15 iterations



(c) 40 iterations

(d) 45 iterations

Figure 2: Comparison of HIO-PIE and PIE using experimental data for 2×2 probe positions.

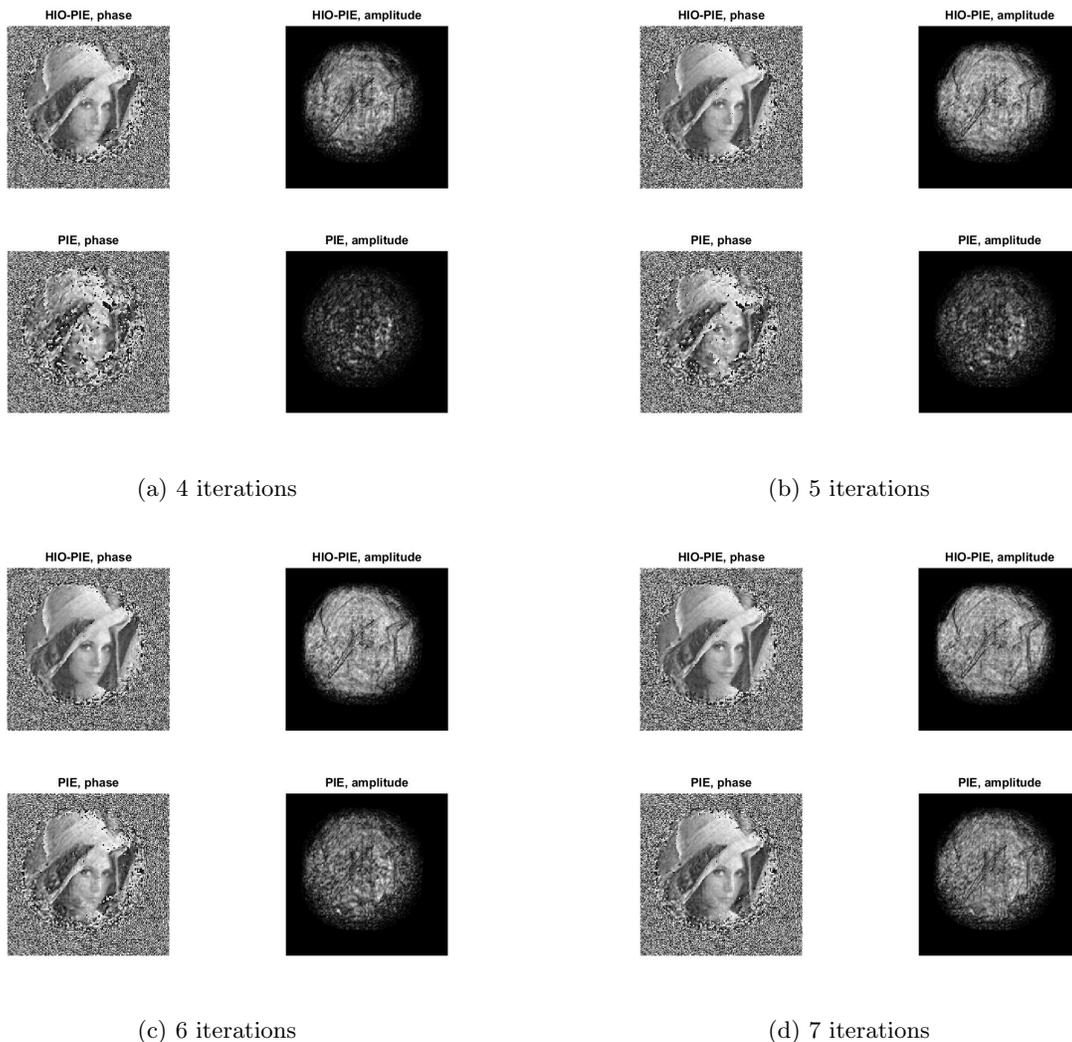


Figure 3: Comparison of HIO-PIE and PIE using experimental data for 3×3 probe positions.

5. CONCLUSION

We have proposed a ptychographical algorithm that combines HIO with PIE by introducing a feedback function per probe position. With simulations, it had been demonstrated previously that the algorithm is noise-robust, and outperforms PIE when few probe positions are used. In a proof-of-principle experiment we have demonstrated that when 2×2 probe positions are used, HIO-PIE gives an object reconstruction significantly faster than PIE. When 2×2 probe positions are used, HIO-PIE still gives an reconstruction faster than PIE, though the difference in the converge rate is smaller.

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