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Phase retrieval in arbitrarily-shaped aperture with the transport-of-intensity equation

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Abstract: Phase is not easy to detect directly as intensity, but sometimes it contains the really desired information. The transport-of-intensity equation (TIE) is a powerful tool to retrieve the phase from the intensity. However, by considering the boundary energy exchange and the whole energy conversation in the field of view, the current popular Fast Fourier transform (FFT) based TIE solver can only retrieve the phase under homogeneous Neumann boundary condition. For many applications, the boundary condition could be more complex and general. A novel TIE phase retrieval method is proposed to deal with an optical field under a general boundary condition. In this method, an arbitrarily-shape hard aperture is added in the optical field. In our method, the TIE is solved by using iterative discrete cosine transforms (DCT) method, which contains a phase compensation mechanism to improve the retrieval results. The proposed method is verified in simulation with an arbitrary phase, an arbitrarily-shaped aperture, and non-uniform intensity distribution. Experiment is also carried out to check its feasibility and the method proposed in this work is very easy and straightforward to use in a practical measurement as a flexible phase retrieval tool.

Keywords: Phase retrieval, transport-of-intensity equation, arbitrarily-shaped aperture, discrete cosine transform, iterative compensation

1. Introduction

Phase information which sometimes contains what we really want is not easy to get directly, as the energy-based optical sensors only detect the intensity. In optical metrology, phase retrieval is a well-known terminology for either optical fringes [1] or optical wavefield [2]. As one of the phase retrieval from intensity techniques for optical wavefield, the famous Transport-of-Intensity Equation (TIE) is continuously researched after proposed by Teague in 1983 [3]. Due to its simple setup and easy implementation, the TIE has been widely used in many applications such as wavefront sensing [4, 5], and electron microscopy [6].

Indeed the TIE is well studied under homogeneous Neumann boundary condition that the phase derivatives in the normal directions at boundary of the field of view (FOV) equal to zero as shown in Fig. 1(a). This condition ensures the optical energy is conserved inside the FOV at different image recording locations. A few applications belong to this condition, for instance, the observation of a center-positioned cell in a “flat wavefront”. Nowadays, the widely used Fast Fourier transform (FFT) based TIE solver works well for phase retrieval in this case [7].

Nevertheless, in many other applications, such as wavefront sensing, it is impossible to have the optical wave satisfy the homogeneous Neumann boundary condition in the FOV. In this case, as shown in Fig. 1(b), the energy inside the FOV is not conserved, as the energy exchanges at the FOV boundary during the recording distance is being changed. The FFT-based TIE solver fails to retrieve the phase under this condition and to solve this problem, Zuo *et al.* [8] suggested adding a rectangular hard aperture to limit the wavefield under test shown in Fig. 1(c) and then to keep the energy conservation. By using Discrete Cosine Transform (DCT), Zuo’s method is able to retrieve the phase under arbitrary boundary conditions and it improves the measuring ability of TIE.

Fig. 1. Energy conservation is required in TIE. (a) Energy is conserved when phase derivatives in the normal directions at boundary edge of FOV $d\phi/dn = 0$. (b) Energy is not conserved when $d\phi/dn \neq 0$. (c) A hard aperture is added in the optical wavefield to make sure the energy conservation.

However, in practice it is quite challenging to add an aperture whose shape is exactly a rectangle, due to the difficulty in aperture fabrication and system alignment, or the other existing pupils (*e.g.* telescopes) obstructing the aperture shape to be a rectangle. Consequently, the performance of Zuo's method may be limited in real applications.

In this work, we present a new method to solve the TIE with a hard aperture (in the case of Fig. 1(c)) but the aperture shape is arbitrary. As a result, the difficulty of aperture fabrication and system alignment can be significantly reduced. The proposed method is extremely flexible for real applications.

2. Method

Let's introduce our method from the famous TIE [3], which describes a paraxial light beam propagating along z axis as

$$-k \frac{\partial I(\mathbf{r})}{\partial z} = \nabla \cdot [I(\mathbf{r}) \nabla \phi(\mathbf{r})], \quad (1)$$

where $I(\mathbf{r})$ and $\phi(\mathbf{r})$ are the intensity and phase at the position $\mathbf{r}$ representing the 2D spatial coordinate (x, y) , k is the wave number $2\pi/\lambda$. Here we define the left hand side of Eq (1) as

$$J := -k \frac{\partial I}{\partial z}. \quad (2)$$

Following the suggestion by Teague [3], an auxiliary function ψ is introduced with satisfying

$$\nabla \psi = I \nabla \phi. \quad (3)$$

Then the TIE is converted to a Poisson equation

$$\nabla^2 \psi = J. \quad (4)$$

It is worthy to note, in order to obtain Eq.(3) and Eq.(4), the "Teague assumption" is implied that the Poynting vector $I \nabla \phi$ should be conservative [9].

This Poisson equation can be solved with a DCT-based solver, which flips the matrices in advance. The flipped matrix J_F can be calculated by

$$J_F = \begin{bmatrix} J(x, y), & J(-x, y) \\ J(x, -y), & J(-x, -y) \end{bmatrix}. \quad (5)$$

Then the flipped auxiliary function ψ_F can be solved by

$$\psi_F = \text{FFT}^{-1} \left\{ \frac{-4\pi^2 (u^2 + v^2) \cdot \text{FFT} \{J_F\}}{\left[-4\pi^2 (u^2 + v^2) \right]^2 + \xi} \right\}, \quad (6)$$

where (u, v) are coordinates in spatial frequency domain, ξ is a regularization parameter to avoid the denominator being zero. The phase derivatives can be calculated as

$$\begin{cases} \frac{\partial \phi_F}{\partial x} = \frac{\text{FFT}^{-1} \{ j \cdot 2\pi u \cdot \text{FFT} \{ \psi_F \} \}}{I_F} \\ \frac{\partial \phi_F}{\partial y} = \frac{\text{FFT}^{-1} \{ j \cdot 2\pi v \cdot \text{FFT} \{ \psi_F \} \}}{I_F} \end{cases}, \quad (7)$$

where the intensity I_F is calculated by firstly filling the intensity I outside the aperture with the average intensity inside to get I_a , and then evenly flipping I_a as

$$I_F = \begin{bmatrix} I_a(x, y), & I_a(-x, y) \\ I_a(x, -y), & I_a(-x, -y) \end{bmatrix}. \quad (8)$$

Then the flipped phase can be calculated through

$$\phi_F = \text{FFT}^{-1} \left\{ \frac{j \cdot 2\pi u \cdot \text{FFT} \left\{ \frac{\partial \phi_F}{\partial x} \right\} + j \cdot 2\pi v \cdot \text{FFT} \left\{ \frac{\partial \phi_F}{\partial y} \right\}}{\left\{ \left[-4\pi^2 (u^2 + v^2) \right]^2 + \xi \right\} / \left[-4\pi^2 (u^2 + v^2) \right]} \right\} \quad (9)$$

The phase ϕ can be cropped from the flipped phase ϕ_F as the output of the DCT-based TIE solver shown in the box in Fig. 2. However, because the invalid intensity outside the aperture is substituted with the inside average value in I_a (referring to step D in Fig. 2), the implicit “Teague assumption” is unlikely to be satisfied, *i.e.* the Poynting vector $I \nabla \phi$ is not conservative and can be decomposed into a curl-free component and a divergence-free component as Eq. (10) according to the Helmholtz decomposition.

$$I \nabla \phi = \nabla \psi + \nabla \times \boldsymbol{\eta}, \quad (10)$$

where ψ and $\boldsymbol{\eta}$ are a scale potential and a vector potential, respectively. The next job is to reduce the error from the curl effect by iterative compensations [9, 10]. The implementation details are illustrated in Fig. 2.

Fig. 2. An iterative DCT-based TIE solver is illustrated for phase retrieval with an arbitrarily-shaped hard aperture.

The process can be described as the following procedures.

Step 1: Solve the TIE by the DCT-based TIE solver with inputs of measured J and I for the initial phase value ϕ_0 . Set the iteration number $n = 0$.

Step 2: Update the $n = n+1$. Calculate the difference between the measured J with the estimated one through

$$\Delta J_n = J - \nabla \cdot (I \nabla \phi_{n-1}). \quad (11)$$

Step 3: Solve TIE by the DCT-based TIE solver with ΔJ_n and I as the input for phase compensation amount $\Delta \phi_n$.

Step 4: Compensate the phase $\phi_n = \phi_{n-1} + \Delta \phi_n$

Step 5: If n reaches the preset maximum iteration number or either $\Delta \phi_n$ or ΔJ_n is smaller than the threshold for each, the loop terminates and go to Step 6. Otherwise, go back to Step 2 and continue the loop.

Step 6: Crop the compensated phase ϕ_n with the aperture and maintain the values inside the aperture for the final phase ϕ .

3. Simulation

A simulation is carried out to verify the proposed method. The CCD FOV is $512\mu\text{m} \times 512\mu\text{m}$ with 256×256 sampling points in simulation. An irregular aperture is simulated to enhance the complexity. The aperture shape is a combination of a knife edge and an ellipse with its central region blocked as shown in Fig. 3(a) and expressed as (unit: mm)

$$\begin{cases} x^2 + y^2 - 0.3xy < 4096\sqrt{2} \times 10^{-5} \\ y > 1024\sqrt{2} \times 10^{-4} \\ \sqrt{x^2 + y^2} < 512\sqrt{2} \times 10^{-4} \end{cases}. \quad (12)$$

The non-uniform intensity is distributed as

$$I(x, y) = \exp\left(-\frac{x^2 + y^2}{2 \times 0.18^2}\right). \quad (13)$$

The intensity inside aperture at focus position is captured as Fig. 3(b). The true phase distribution can be theoretically arbitrary and here not purposely set as

$$\phi(x, y) = 10x^2 - 10y^2 + 0.7x + 2y + 0.82. \quad (14)$$

The true phase distribution is shown in Fig. 3(c). Please note that only the values inside the aperture are of interest. Two oppositely defocused (± 0.5 mm) images are shown in Fig. 3(d) and (e).

Fig. 3. TIE through a hard aperture, which is in an irregular shape (a), is simulated with intensity at focus (b), true phase (c), intensity at $z = -0.5$ mm (d), intensity at $z = 0.5$ mm (e), and $\partial I / \partial z$ (f).

Once the intensity images are obtained, the intensity derivative $\partial I / \partial z$ can be calculated and shown in Fig. 3(f). In simulation the wave length $\lambda = 633$ nm. The calculated J and the filled intensity I_a , shown in Fig. 4 (a) and (b) are used as the inputs to the DCT-based TIE solver, which results in the initial phase ϕ_0 shown in Fig. 4(c).

Fig. 4. With the inputs of the calculated J (a) and filled intensity I_a (b), the DCT-based TIE solver can estimate an initial phase (c).

After employing the proposed iteration, the standard deviation (STD) of phase error inside aperture is reduced as shown in Fig. 5. Accuracy of the retrieved phase is significantly improved from the initial phase errors [Fig. 5(a)] with STD = 0.095 rad to STD = 0.005 rad [Fig. 5(b)] in only 10 iterations.

Fig. 5. The proposed iteration effectively reduces the errors of phase estimation from the initial errors (a) down to the updated ones (b), and the phase in FOV (c) and inside the aperture (d) can be retrieved as results.

The estimated phase distribution in the complete FOV after iterative compensations is shown in Fig. 5(c). Of course, only the values inside the aperture are desired and reliable. The final phase distribution shown in Fig. 5(d) with its corresponding error distributed in Fig. 5(b) indicates the high accuracy of the proposed method.

4. Experiment

In order to demonstrate its feasibility in practice, the proposed method is also tested with a set of real TIE data. As illustrated in Fig. 6, an inverted bright-field microscope (Olympus IX71) attached with a tunable lens based TIE (TL-TIE) system is used to acquire the intensity images in and out of focus. The pixel size of the CCD (Imaging Source DMK 41AU02 1280×960) is 4.65 μm . In the experiment, the wavelength is 550 nm.

Fig. 6 The TIE experiment is implemented by using an inverted bright-field microscope and a tunable lens based TIE module with placing an aperture at the image plane.

The specimen is a piece of microlens array. At its image plane, a rectangle-like aperture is placed. The intensity at focus is shown in Fig. 7(a) with its intensity histogram in Fig. 7(b), which indicates it is easy to set an intensity threshold to separate the regions in and out of aperture. By varying the focal length of the tunable lens, the defocused images are obtained at equivalent defocusing distances of $-550 \mu\text{m}$ in Fig. 7(b) and $+550 \mu\text{m}$ in Fig. 7(c), sequentially. The intensity derivative $\partial I/\partial z$ is shown in Fig. 7(d).

Fig. 7. The experimentally captured intensity at focus (a) with its histogram (b), and the intensity at $-550 \mu\text{m}$ (c) and $+550 \mu\text{m}$ (d) as well as their intensity derivative $\partial I/\partial z$ (e).

In order to have a benchmark to compare the accuracy, Zuo's method [8] is implemented by using the data in a rectangular region $\bar{\Omega}$ (within dashed yellow lines) including the aperture boundary shown in Fig. 8(a). Due to the characteristic of Zuo's method, the phase reconstruction happens within a slightly smaller rectangular region Ω (within solid green lines) instead. The phase retrieved with Zuo's method is in Fig. 8(b), which will be the benchmark for the following comparison.

Fig. 8. Zuo's method uses the information in "data region $\bar{\Omega}$ " to retrieve phase in reconstruct region Ω (a), and its result (b) is used as a benchmark to judge the results from classical FFT-based TIE solver (c) and the proposed method (d). The phase retrieved with the proposed method is much closer to Zuo's result (f) than the classical one does (e).

The classical FFT-based TIE solver is also implemented to retrieve the phase within the rectangular region Ω (within solid green lines), whose result is shown in Fig. 8(c). The phase result within the whole aperture shown in Fig. 8(d) is retrieved by the proposed method after 6 iterations. The difference between phase results from classical FFT-based method and Zuo's method is very large (STD = 21.11 rad) as shown in Fig. 8(e), and Fig. 8(f) shows the phase difference between the proposed one with Zuo's is much smaller with STD = 1.25 rad only. The comparison indicates the proposed method can retrieve a more accurate phase result than the classical FFT-based method does when the homogeneous Neumann boundary condition is not satisfied.

5. Discussion

Although the phase retrieved by the proposed method is similar to that by Zuo's method, it is very worthy to note their difference in data processing. Theoretically, Zuo's method requires the rectangular aperture is recorded with its boundaries parallel to the pixel coordinates in order to take the DCTs in its selected the rectangular "data region" and "reconstruction region". Furthermore, the size of "reconstruction region" is determined based on the defocusing distance and wavelength in use. As a result, it may require some experience to select proper regions for a good result in practice. On the other hand, the method proposed in this work can handle apertures in arbitrary shapes and does not care about the relationship between aperture boundary and CCD pixel coordinates. Moreover, the proposed method treats the input images as a whole piece of data without cutting any regions in advance, and consequently it is pretty straightforward to employ the proposed method in practice.

6. Conclusion

In this work, an iterative DCT-based TIE solver is proposed to accurately retrieve the phase information through adding a hard aperture on the tested optical field. In hardware, the added aperture can be in an arbitrary shape which results in a low requirement on aperture fabrication and alignment. In data processing, the procedure is extremely automatic and easy to use. These features of the proposed method significantly enhance the flexibility of TIE measurement with hard aperture in real applications.

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