IMPROVING ACQUISITION SPEED OF X-RAY PTYCHOGRAPHY THROUGH SPATIAL UNDERSAMPLING AND REGULARIZATION

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ABSTRACT

X-ray ptychography is one of the versatile techniques for nanometer resolution imaging. The magnitude of the diffraction patterns is recorded on a detector, and the phase of the diffraction patterns is estimated using phase retrieval techniques. Most phase retrieval algorithms make the solution well-posed by relying on the constraints imposed by the overlapping region between neighboring diffraction pattern samples. As the overlap between neighboring diffraction patterns reduces, the problem becomes ill-posed, and the object cannot be recovered. To avoid the ill-posedness, we investigate the effect of regularizing the phase retrieval algorithm with image priors for various overlap ratios between the neighboring diffraction patterns. We show that the object can be faithfully reconstructed at low overlap ratios by regularizing the phase retrieval algorithm with image priors such as Total-Variation prior and Structure Tensor Prior. We also show the effectiveness of our proposed algorithm on real data acquired from an IC chip with a coherent X-ray beam.

Index Terms— Ptychography, Phase-retrieval, Regularization, Automatic Differentiation

1. INTRODUCTION

X-ray ptychography has become one of the most popular techniques to achieve resolutions of up to a few nanometers in imaging objects. The ptychography technique was first proposed by Hoppe [1] in 1969 and was then further developed experimentally and algorithmically in the 2000s [2, 3, 4, 5]. This technique has both research and industrial applications in various fields such as biological imaging and material sciences. In this technique, a focused, coherent X-ray probe beam interacts with the object to be imaged and produces an exit wavefront. The exit wavefront propagates to the far-field, and the propagated wavefront is approximated by the Fourier transform of the exiting wavefront (see Fig. 1). A 2D detector is placed in the far-field, which records the intensities of the propagated wavefront. As the probe beam is narrow, it interacts with only a small part of the object each time, and it scans across the entire object in steps. During each scan, the detector only records the square of the magnitude of the Fourier transform of the wavefront exiting from the object, whereas the phase is completely lost. Therefore, recovering the object field requires solving an ill-posed phase-retrieval problem, where one has to reconstruct the complex object field given only the magnitude of its Fourier transform [6, 7, 8, 9]. To enforce an unique solution for phase-retrieval, sufficient overlap between successive scan points of the probe beam is necessary [10].

Scanning the object with enough overlap between successive scan points typically leads to very long acquisition times and inhibits high throughput scanning. In image processing, ill-posed problems are typically regularized by imposing prior knowledge about the image to be restored. Several image priors have been proposed in the literature ranging from signal-agnostic priors to signal-specific priors. In this work, we propose to regularize the solution to the phase retrieval algorithm by imposing constraints arising from the prior knowledge about the object to be estimated. We explore the use of regularizers that are well suited for the reconstruction of an integrated circuit (IC) chip from X-ray diffraction measurements.

Many phase retrieval algorithms attempt to iteratively estimate the object by imposing the constraints observed in the overlap region and the measurement observed in the diffraction patterns. Many gradient descent based algorithms have
also been proposed, which rely on manually derived closed-form expressions for the gradient of the cost-function [6, 11, 12]. Very recently, alternative algorithms have been introduced which perform gradient descent using automatic differentiation of the cost-function [13, 14, 15]. These algorithms have the flexibility of using complex but differentiable terms in the cost function and can also provide easy hardware acceleration on the GPU. We adopt the automatic differentiation based ptychographic phase retrieval algorithm [13, 14] for investigating the role of image priors in regularizing the ill-posedness. Specifically, we investigate two different image prior models a) Total-Variation prior (TV) [16] and b) Structure Tensor Prior (STP) [17]. We show that the 2D object fields of an IC chip can be faithfully reconstructed at low overlap ratios by regularizing the phase retrieval algorithm with image priors such as Total-Variation prior [16] and Structure Tensor Prior (STP) [17]. It has been previously shown that data-driven prior models can help regularize the ill-posed phase retrieval problem when the overlap ratio is low [18, 19] in Fourier ptychography. Here, we investigate the impact of using various prior models for regularizing the phase retrieval problem for X-ray ptychography under various overlap ratios. Note that our algorithm tackles an ill-posed problem of reconstructing the complex probe beam, in addition to the object field.

2. REGULARIZED X-RAY PTYCHOGRAPHY

In X-ray ptychography, a focused, coherent X-ray probe beam \( P(r) \) interacts with a complex object \( O(r) \). The X-ray beam exits the object as a wavefront \( \psi(r) \) and then propagates to the far-field, which can be approximated by the Fourier-transform. A detector is placed at the far-field, which records the diffraction pattern \( I(k) \) of the far-field propagated wavefront \( \psi(r) \). Mathematically, the ptychographic imaging process is modeled as,

\[
\psi_i(r) = P(r - r_i) \odot O(r)
\]

(1)

\[
I_i(k) = |\mathcal{F}[\psi_i(r)]|^2
\]

(2)

where \( r_i \) is the current position of the coherent probe beam, \( \odot \) indicates pointwise multiplication, and \( \mathcal{F} \) denotes the Fourier-transform from the real-space co-ordinates\((r)\) to the reciprocal-space co-ordinates\((k)\). In this problem, the quantities of interest to be estimated are the probe beam \( P(r) \) and the complex object \( O(r) \). Let \( \hat{P}(r) \) and \( \hat{O}(r) \) be the estimates of the original signal. Following the work of Ghosh et al. [13], we formulate the estimation of these quantities as the minimization of the objective function defined as

\[
\mathcal{E}_o = \frac{1}{M} \sum_{i \in M} \left( |\mathcal{F}[\hat{P}(r - r_i) \odot \hat{O}(r)]| - \sqrt{I_i(k)} \right)^2
\]

(3)

where \( M \) is the number of probe positions. In each iteration, a batch of \( M \) probe positions is sampled and the objective \( \mathcal{E}_o \) is computed according to eq. (3). The energy \( \mathcal{E}_o \) is minimized using gradient descent steps where the gradients are obtained using an automatic differentiation algorithm [13, 14].

2.1. Object Regularization

In this work, we mainly consider ptychographic imaging of IC chips with nanometer resolution. We know for a fact that such objects, when imaged, have a piecewise smoothness property, and hence we consider prior models that impose such a constraint on the estimated phase and magnitude of the object. Particularly, we consider two prior models a) Total Variation prior (TV) [16] and b) Structure Tensor Prior (STP) [17]. As the object \( O \) to be estimated is a complex field, we impose the prior models separately on the object-magnitude \(|O|\) and the object-phase \(\angle O\). TV prior has been widely used in the field of image processing and is defined as

\[
\mathcal{E}_{pTV} = \sum_i \|\nabla_i |O|\|_2 + \sum_i \|\nabla_i \angle O\|_2
\]

(4)

where \( \nabla_i \) is the finite difference image gradient operator. STP [17] imposes a sparsity constraint on the eigenvalues of the structure tensor \( S_k \). The structure tensor \( S_k \) is defined as \( S_k = K \ast \{ H(1) \} \), where \( K \) is a gaussian smoothing kernel, \( \ast \) denotes convolution and \( H(1) \) is the pixel-wise Hessian of the image \( I \). Let \( \lambda_k^+ \geq \lambda_k^- \geq 0 \) be the eigen values of \( S_k \), then the cost for the STP is defined as,

\[
\mathcal{E}_{pSTP} = \frac{1}{N} \sum_{i=1}^{N} |\lambda_i^+| + |\lambda_i^-|
\]

(5)

Besides regularizing the phase retrieval algorithm with image prior we also propose to exploit correlations between the phase and the magnitude estimations. To do that, we employ the cross-channel prior proposed by Heide et al. [20].

Fig. 1. Ptychographic object acquisition model: A complex probe beam \( P \) interacts with a complex object \( O \) to produce an exit wavefront \( \psi \). The wavefront \( \psi \) propagates to the far-field where the magnitude of the wavefront is recorded on the sensor. The probe beam scans the entire object in steps with the scanning region overlapping between neighboring samples.
The cross-channel prior \[20\] over the object magnitude \(|O|\) and the object-phase \(\angle O\) is defined as
\[
E_p^{CC} = \| \nabla \angle O \odot |O| - \nabla |O| \odot \angle O \|_1
\]
(6)
where \(\nabla\) denotes the finite difference gradient operator and \(\odot\) represents element-wise multiplication.

### 2.2. Probe Retrieval

In a ptychographic imaging experiment, it is difficult to know the exact complex beam profile of the probe \(P(r)\). In [13], the authors initialize the probe \(P^0\) as
\[
P^0 = \mathcal{F}^{-1}\left\{ \frac{1}{M} \sum_{i=1}^{M} \sqrt{I_i(k)} \right\},
\]
(7)
and update it after each iteration of the object reconstruction algorithm. We follow a similar approach to estimate the probe initialization as in eq. (7). Additionally, the probe \(P^0\) is Fresnel propagated by a few micrometers to obtain a defocused probe. We also know that the magnitude of the beam profile varies smoothly across the probe. We define a cost \(E^p_{pr}\) that enforces a smoothness constraint on the probe magnitude to our overall objective. We define \(E^p_{pr} = \| \nabla |P| \|_2\), where \(|P|\) denotes the magnitude of the estimated probe. Overall our objective becomes,
\[
O, P = \arg \min_{O, P} \mathcal{E}_o + \lambda_1 \mathcal{E}_p^x + \lambda_2 \mathcal{E}_p^{CC} + \lambda_3 \mathcal{E}_p^{pr}
\]
(8)
where \(x \in \{TV, STP\}\) and \(\lambda_1, \lambda_2, \lambda_3\) are the regularization hyper-parameters.

### 3. EXPERIMENTS

To demonstrate our technique, we perform simulation experiments, where we consider a complex object \(O \in \mathbb{C}^{192 \times 192}\), a projection of a chip, as shown in Fig. 2a. We simulate the diffraction patterns using Eqs. (1) and (2), where probe \(P \in \mathbb{C}^{64 \times 64}\), whose magnitude is a gaussian kernel with a standard deviation of 12 pixels. The phase of the probe is obtained from the reconstruction of a real object using the algorithm proposed in [15].

The optimization is initialized with values of \(|O|\) and \(\angle O\) uniformly drawn from \([0.9, 1.0]\) and \([-0.1, 0.1]\), respectively. The probe is initialized as described in eq. (7). We use Adam optimizer [21] with a batch size of 16, and initial learning rates of 0.1 and 0.01 for the object and probe respectively. The optimization algorithm is implemented using the PyTorch [22] automatic differentiation framework.

#### 3.1. Probe smoothness

We investigate the effectiveness of imposing the probe smoothness prior on the estimated probe. Diffraction patterns are simulated with a step size of 8 pixels or an overlap of 78\%. For the case of probe smoothness loss, we minimize the objective \(E = \mathcal{E}_o + \lambda \mathcal{E}_p^{pr}\) with \(\lambda = 0.01\). In Fig. 2b and 2c, we show the reconstructed object without and with the probe.

#### 3.2. Cross channel (CC) prior

To investigate the effectiveness of the cross-channel prior, we simulate diffraction patterns with a step size of 12 pixels (overlap ratio of 57\%). We compare the effectiveness of
the cross-channel prior with that of using only the probe-smoothness prior and using no prior at all. For the case of probe smoothness loss, we minimize the same objective as in Sec. 3.1 and for the case of the cross-channel prior we minimize the objective $E = E_o + \lambda_1 E_{pr} + \lambda_2 E_{CC}$ where $\lambda_1 = \lambda_2 = 0.01$. In Fig. 3, we show the reconstructed object using no prior, probe smoothness prior alone, and using both the probe smoothness prior and the cross-channel prior. We observe that the cross-channel prior regularizes the solution well and estimates an artifact-free object.

3.3. Gradient Sparsity Regularization

Finally, we investigate the effect of imposing gradient sparsity on the estimated object. We compare two different prior models a) TV prior and b) Structure Tensor Prior. We minimize the objective $E = E_o + \lambda_1 E_{pr} + \lambda_2 E_{CC} + \lambda_3 E_p$ where $x = TV$ or $x = STP$. We simulate the diffraction patterns for 4 different overlap ratios of 78%, 57%, 36% and 15%. We set $\lambda_1 = \lambda_2 = 0.01$ for object reconstruction for all the overlap ratios. We set $\lambda_3 = 0.005$ for overlap ratios of 78%, 57% and $\lambda_3 = 0.01$ for overlap ratios of 36% and 15%. We show the reconstructed objects with TV prior and STP prior in Fig. 4. For comparison, we show the objects reconstructed with the cross-channel prior as well for all the overlap ratios. We observe that the cross-channel prior fails to regularize the solution at very low overlap ratios. However, gradient sparsity inducing priors such as TV and STP can recover the major details of the object at very low overlap ratios. We also provide a quantitative comparison of the estimated objects in Fig 5.

3.4. Real data

We demonstrate the effectiveness of the proposed regularization methods on real data that were obtained from [23]. It consists of 175 diffraction patterns, recorded in the region of interest of the IC chip following the Fermat spiral trajectory [24]. The scan points have an average spacing of 0.7µm. We artificially introduce undersampling by holding out some of the captured diffraction patterns from the reconstruction algorithm. We consider three cases where the object is reconstructed using a) all the 175 samples, b) only 99 samples, and c) only 61 samples. The undersampling is done by uniformly thinning the set of 175 2-D scan points. We show the object reconstructed from the above three cases without using any prior, using a TV prior, and using STP prior in Fig. 6. We also show the complex object reconstructed under various overlap ratios using ePIE [3], a previously proposed phase retrieval algorithm. ePIE [3] is an iterative greedy algorithm that simultaneously reconstructs both the probe and the object and does not impose any signal prior constraint on the estimated quantities. When the signal prior is not imposed during reconstruction, both our algorithm and ePIE quickly degrade in the reconstruction performance with decreasing overlap ratios. When using the STP and the TV priors, the algorithm is able to recover major details even for very low overlap ratios.

Fig. 5. We show the plot of SSIM of the estimated object phase for different overlap ratios when the object is estimated without any prior, TV prior and the STP prior.

![Figure 5](image)

Fig. 6. We show the phase of the complex object reconstructed using the captured real data. With higher step sizes (indicating low overlap ratios) the object estimate degrades rapidly when no prior is imposed. When using the TV prior or the STP prior the object is recovered properly for low overlap ratios as well.

4. CONCLUSIONS

High throughput scanning in X-ray ptychography requires the overlap between the neighboring scan points to be low. Here, we investigate the ill-posedness of the phase retrieval algorithm for object recovery for various overlap ratios. We introduce regularization of the phase retrieval algorithm by imposing various prior models such as TV, STP, and CC priors. We show that using prior models in the minimization objective can regularize the phase retrieval for very low overlap ratios. When the overlap is high, prior models help in removing the artifacts compared to not using any prior model. For very low overlap ratios, the prior models tend to over-smooth the reconstructed object, and hence better and stronger models can be designed in the future.
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