Regularization for Undersampled Ptychography

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Abstract: Ptychography becomes increasingly ill-posed when the overlap between neighboring scan points is reduced, inhibiting the object reconstruction. Here, we discuss and show reconstructions with low-overlap ratios by regularizing with priors such as Total-Variation and Structure-Tensor-Prior.

1. Introduction

X-ray ptychography is a versatile technique to achieve nanometer resolutions in imaging. It has found several applications in both research and industry, e.g., in biology and material sciences.

In X-ray ptychography, a focused, coherent probe beam $P(r)$ interacts with an object $O(r)$. The resulting wavefront $\psi(r)$ then propagates in free-space to the far-field, which can be approximated by the Fourier-transform of the wavefront. Then a 2D detector measures the intensity of the resulting diffraction pattern. Only a part of the object information can be captured in each measurement due to the limited size of the probe. To image the complete object, the focused beam is scanned across the sample with sufficient overlap between consecutive scan positions. Note that the phase information of the diffraction patterns is lost as only the intensities are recorded. Hence, phase retrieval algorithms are required to recover the original signal $O(r)$. Furthermore, working at nanometer precision, it is not possible to have an accurate measure of the probe. Both object and probe need to be reconstructed, making ptychography especially challenging.

Most phase-retrieval algorithms fix the ill-posedness of the problem by relying on the constraints imposed by the partial overlap of the neighboring scan points. The observed redundancy is required to determine a unique solution to the ill-posed phase retrieval problem. However, scanning with enough overlap between successive scan points leads to long acquisition times that inhibit high throughput scanning. To alleviate this problem, many works in the literature introduce prior knowledge about the original signal as a regularization term.

In this work, we investigate the effect of regularizing the phase retrieval algorithm for several overlap ratios between the neighboring scan points. 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 [1] and Structure Tensor Prior (STP) [2].

2. Method

Mathematically, the ptychographic imaging process is modeled by

$$\psi_i(r) = P(r - r_i) \odot O(r) \ , \quad (1) \qquad I_i(k) = |\mathscr{F}[\psi_i(r)]|^2 \ , \quad (2)$$

where r_i is the current position of the coherent probe beam, $\odot$ indicates pointwise multiplication, and $\mathscr{F}$ denotes the Fourier-transform from the real-space (r) to the reciprocal-space (k). To recover the signal and the probe, we adopt the work proposed by Ghosh *et al.* [3], which uses automatic differentiation to solve the phase retrieval problem by minimizing the following objective function

$$\mathscr{E}_o = \frac{1}{M} \sum_{i \in M} \{ |\mathscr{F}[P(r - r_i) \odot O(r)]| - \sqrt{I_i(k)} \}^2 \ , \quad (3)$$

where M is the number of probe positions. When the overlap between neighboring scan points is low, additional constraints in the form of prior information is necessary. This prior information is imposed on the complex object to be recovered and can be written as an additional energy term $\mathscr{E}_p$. Overall, by minimizing the combined energy $\mathscr{E} = \mathscr{E}_o + \lambda \mathscr{E}_p$ we can recover the complex object $O(r)$.

Here, we consider two prior models a) Total-Variation (TV) [1] and b) Structure Tensor Prior (STP) [2], which are defined as

$$\mathscr{E}_p^{TV} = \sum_i \|\nabla_i O\|_2 \ , \quad (4) \qquad \mathscr{E}_p^{STP} = \frac{1}{N} \sum_{i=1}^{N} |\lambda_i^+| + |\lambda_i^-| \ . \quad (5)$$

where ∇_i is the finite difference image gradient operator. The STP imposes sparsity on the eigenvalues of the structure-tensor S at each pixel of the image O. If λ_i^+ and λ_i^- are the two eigenvalues of the structure tensor S [2]

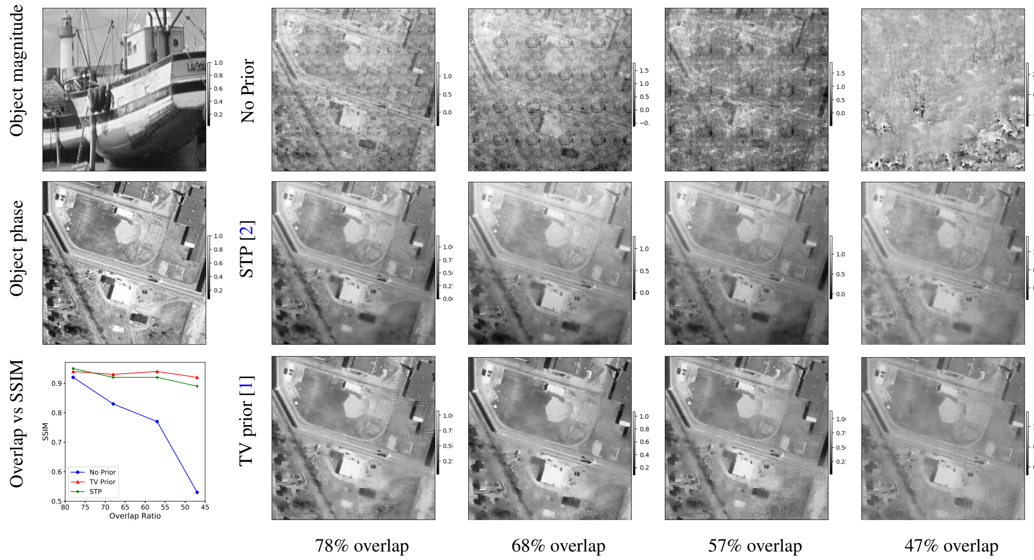

Fig. 1: We show reconstructed object phase for various overlap ratios in ptychographic sampling. We observe that with reduction in overlap ratios the phase cannot be recovered faithfully without additional prior.

at pixel i, then structure tensor prior is defined as the average of the magnitudes of the eigenvalues over the image O as shown in Eq. (5). We refer the readers to [2] for further details regarding structure tensor prior.

To simulate diffraction patterns, we use two natural images as the magnitude and the phase of our complex object. The magnitude of the probe is initialized as a gaussian kernel of size 256×256 with a standard deviation of 64 pixels. We obtain a probe used to reconstruct an object from real experimental data using the algorithm proposed in [4]. The phase map of this probe is used as the probe phase to simulate the diffraction patterns. The diffraction patterns are simulated using the forward model shown in Eq. (1). We empirically choose $\lambda = 0.01$ as our regularization hyper-parameter in all our experiments. We show the reconstructed objects obtained from imposing no prior, TV prior and STP for various overlap ratios in Fig. 1. We observe that as the overlap ratio reduces, the object reconstruction becomes increasingly ill-posed. To tackle this, we need to impose the prior knowledge on the reconstructed object. Image priors such as TV prior and STP can regularize the solution obtained during the iterative object reconstruction. We can see from Fig. 1, that this regularization helps in obtaining consistent results for various overlap ratios. However, in the case of a low overlap ratio and without regularization, the object cannot be estimated faithfully.

3. Discussion and Outlook

We demonstrate that highly undersampled pytchography data can be reconstructed with high fidelity using appropriate priors. Further research will verify this hypothesis with experimental data. Furthermore, to achieve scanning with very low overlap between neighboring scan points, the development of a more powerful reconstruction algorithm is required.

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