Phase Retrieval with Holography and Untrained Priors: Tackling the Challenges of Low-Photon Nanoscale Imaging

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Abstract
Phase retrieval is the inverse problem of recovering a signal from magnitude-only Fourier measurements, and underlies numerous imaging modalities, such as Coherent Diffraction Imaging (CDI). A variant of this setup, known as holography, includes a reference object that is placed adjacent to the specimen of interest before measurements are collected. The resulting inverse problem, known as holographic phase retrieval, is well-known to have improved problem conditioning relative to the original. This innovation, i.e. Holographic CDI, becomes crucial at the nanoscale, where imaging specimens such as viruses, proteins, and crystals require low-photon measurements. This data is highly corrupted by Poisson shot noise, and often lacks low-frequency content as well. In this work, we introduce a dataset-free deep learning framework for holographic phase retrieval adapted to these challenges. The key ingredients of our approach are the explicit and flexible incorporation of the physical forward model into an automatic differentiation procedure, the Poisson log-likelihood objective function, and an optional untrained deep image prior. We perform extensive evaluation under realistic conditions. Compared to competing classical methods, our method recovers signal from higher noise levels and is more resilient to suboptimal reference design, as well as to large missing regions of low frequencies in the observations. To the best of our knowledge, this is the first work to consider a dataset-free machine learning approach for holographic phase retrieval.

1. Introduction
Phase retrieval is a nonlinear inverse problem that arises ubiquitously in imaging sciences, and has gained much recent attention (Shechtman et al., 2015). In this work we focus on a practical instance of the problem that arises in Coherent Diffraction Imaging (CDI). Here, holographic phase retrieval consists of recovering an image $X_0 \in \mathbb{R}^{m \times n}$ from a set of squared Fourier transform magnitudes

$$Y = |F(X_0 + R_0)|^2,$$

where $F$ denotes an oversampled Fourier transform operator and $R_0 \in \mathbb{R}^{m \times n}$ is a known reference image whose support does not intersect the support of $X_0$. The known reference image $R_0$ distinguishes holographic phase retrieval from the (classical) phase retrieval setting, where the goal is to
recover $X_0$ from $|F(X_0)|^2$ alone. We focus entirely on the holographic version of the problem in realistic conditions: with high noise levels and missing low-frequency data. The advantage provided by the holographic reference is briefly illustrated on Figure 1.

Figure 1: The advantage of using a reference for phase retrieval at $N_p = 1$ photon/pixel. Two algorithms, HIO and our HolOpt-P, are applied to reconstruct from Fourier magnitude data of image alone (classical phase retrieval), and image with reference (holographic phase retrieval). Comparing between algorithms, observe the higher-quality reconstruction when the reference is present. (VIRUS image courtesy of Ghigo et al. (2008))

In the remainder of this introduction we will situate this problem in the context of Coherent Diffraction Imaging, review related works, and list our contributions. Section 2 describes our setup in detail, and Section 3 our reconstruction strategy. In Section 4, we describe extensive experiments and compare to several baseline methods. Section 5 concludes with a general discussion.

1.1. Holographic Coherent Diffraction Imaging and phase retrieval

Coherent Diffraction Imaging (CDI) is a scientific imaging technique used for resolving nanoscale scientific specimens, such as viruses, proteins, and crystals (Miao et al., 1999). In CDI, an image is sought to be reconstructed from X-ray diffraction measurements recorded on a CCD detector plane. By the far-field approximation of optical theory, these measurements are approximately proportional to the squared magnitude values of the Fourier transform of the electric field within the diffraction area. Thus, the specimen structure (e.g., its electron density) can be determined, in principle, by solving the phase retrieval problem. Holographic CDI is a popular setup to perform CDI experiments in which the object undergoing diffraction physically consists of a specimen together with a “reference”, i.e. a portion of the object a priori known. This setup is illustrated in Figure 2. The inclusion of a reference in the CDI setup both enhances the quality of image reconstruction, and greatly simplifies the analysis and solution of the corresponding phase retrieval problem (Marchesini et al., 2008; Guizar-Sicairos and Fienup, 2007; Barmherzig et al., 2019).

Nevertheless, holographic CDI remains challenging in practice. Due to the quantum mechanical nature of photon emission and absorption, CDI measurements are inherently corrupted by Poisson shot noise. The severity of this noise corruption is inversely proportional to the strength of the X-ray source in use, which is in turn quantified via $N_p$, the number of photons per pixel reaching the detector plane. Nanoscale applications of CDI often necessitate imaging in the low-photon regime, where measurements are highly corrupted by noise. CDI measurements are also typically lacking low-frequency data, due to the presence of a beamstop apparatus which occludes direct measurement of these values (He et al., 2015; Latychevskaia, 2019; Barmherzig et al., 2020).
The holographic phase retrieval problem is commonly solved by inverse filtering (Gabor, 1948; Kikuta et al., 1972), which amounts to solving a structured system of linear equations. While straightforward, this method is not well-suited for noisy data. Wiener filtering (Gorkhover et al., 2018) is a variant on this method with some denoising ability. Yet Wiener filtering is derived to account for an additive noise model — an assumption which is not true for Poisson shot noise at low photon counts, and only holds as an approximation at high photon count levels (Salditt et al., 2020). Moreover, these methods do not account explicitly for missing low-frequency data, and require a minimum separation between the specimen and the reference objects, the holographic separation condition (see Section 4.3). The most popular algorithm for the classical phase retrieval problem is the Hybrid Input-Output (HIO) algorithm (Fienup, 1978), which is based on an alternating projection scheme. This method can be modified to the holographic setting by adding an additional projection step to enforce the reference constraints, which greatly improves the algorithm’s performance (Barmherzig et al., 2019).

1.2. Related work

Machine learning for inverse problems Increasing research effort has been devoted to addressing inverse problems, even beyond phase retrieval, with deep learning approaches (see Ongie et al. (2020) for a recent review). Supervised strategies can be broadly divided into four main categories: end-to-end methods, (e.g. McCann et al. (2017)), “unrolling” algorithms (e.g. Meinhardt et al. (2017)), pretrained image denoisers (e.g. Romano et al. (2017)), and learned generative models as highly informative priors (e.g. Tramel et al. (2016)). All of these approaches require a training set, containing either matched signal-observation pairs or simply typical signals, with a large number of data points. The reconstruction improves drastically when this information is available. However, it is often unrealistic to assume such prior knowledge on the measured signal. Recently, for the reconstruction of images, it was found that untrained generative neural networks with appropriate architectures can still be efficient priors (Lempitsky et al., 2018; Heckel and Hand, 2019). By adjusting their parameters to fit a single output observation, they do not require a training set, and instead encourage naturalistic images due to architecture alone. In this paper we focus on the last approach, as it is widely applicable to image data and satisfies our requirement of applicability in a realistic setting.

Machine learning for phase retrieval More specifically, several variants of the phase retrieval problem have received attention in the context of machine learning for inverse problems. Compressive Gaussian phase retrieval, where one observes the amplitude of random complex Gaussian projections of the signal, is a popular setting in the machine learning community. It is easier than the Fourier phase retrieval problem and often more amenable to theoretical analysis (see e.g. Aubin et al. (2020)). For this version of the problem, trained generative models such as Generative Adversarial Networks (Shamshad and Ahmed, 2018; Hand et al., 2018), as well as untrained priors (Jagatap and Hegde, 2019), were found to be very effective on machine learning toy datasets. An increasing number of works now consider the more realistic problem of Fourier phase retrieval. Using pre-trained Gaussian denoisers and iterative algorithms, Deep-prior-based sparse representation (Shi et al., 2020), prDeep (Metzler et al., 2018) and Deep-ITA (Wang et al., 2020b), are solutions robust to noise in the case where the corruption is small enough to be approximately Gaussian. The end-to-end solution investigated by Uelwer et al. (2019) features some robustness to Poisson shot noise, but struggles to generalize to complicated datasets. Meanwhile, the “physics-informed”
architecture of Goy et al. (2018), which includes information about the data generating process, is shown to perform well on realistic signals at very low photon counts, but requires a few thousand training examples. Closer to our work, Wang et al. (2020a) proposed a U-net and Bostan et al. (2020) tested the deep decoder, both untrained neural networks, for Fourier phase retrieval, but did not consider the holographic setting. To the best of our knowledge, Rivenson et al. (2018) is the only proposition considering holography, showing that deep neural networks trained end-to-end on a dataset of a few hundred images lead to state-of-the-art performance.

Other optimization approaches The use of auto-differentiation for Fourier phase retrieval was initiated by Jurling and Fienup (2014), while the convenience of deep learning packages was exploited later (Nashed et al., 2017; Kandel et al., 2019). Thibault and Guizar-Sicairos (2012) derived conjugate gradients to optimize the likelihood for classical (non-holographic) CDI, following either the Poisson or the Euclidean metric. Recently, Barmherzig and Sun (2020) pointed at the potential of likelihood optimization for holographic phase retrieval.

1.3. Our contributions

We address the holographic phase retrieval problem in the low-photon regime using a Poisson maximum likelihood framework and recent insights in machine learning for inverse problems. Our strategy combines three key ideas: (i) a realistic physical noise model for CDI, (ii) auto-differentiation and efficient optimization readily available in a package like PyTorch (Paszke et al., 2019), and lastly (iii) the option to add a neural network prior. We (a) compare these methods to baselines, exploring several experiment challenges; (b) demonstrate significant improvements at different noise levels; (c) investigate the impact of missing low-frequency data on our methods, and show that ours are more robust than baseline methods; (d) investigate the impact of the distance between object image and reference image on reconstruction quality, showing that our proposed method can easily deal with distances below the holographic separation condition; and (e) vary the oversampling rate of observation, observing a graceful degradation of reconstruction with decreasing samples. Finally, we (f) provide a Python package\(^1\) to run our implementation.

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\(^1\) URL to download package and experiments code
2. Holographic CDI Setup

The data generation process mimics the key components of a holographic diffraction experiment as realistically as possible, namely by including two crucial ingredients: the Poisson shot noise model and the beamstop occluding low-frequency measurements.

Coherent diffraction imaging Let $Z \in \mathbb{R}^{m \times n}$ represent a real $m \times n$-pixel image. As explained in Section 1.1, the recorded CDI measurements can be approximated by the square of the oversampled Fourier transform magnitude of the object image. Here, we assume an oversampling factor of two, which is the minimum oversampling factor theoretically required for perfect reconstruction in the noiseless setting (Hayes, 1982). Let $F: \mathbb{R}^{m \times n} \rightarrow \mathbb{C}^{2m \times 2n}$ be the doubly oversampled discrete Fourier transform operator. $F(Z)$ can be implemented as the discrete Fourier transform of a zero-padded version of $Z$. Let $\hat{Z} = \left( \begin{array}{c} Z \\ 0 \\ 0 \end{array} \right) \in \mathbb{R}^{2m \times 2n}$. Then let $F(Z) = \mathcal{F}(\hat{Z})$, where $\mathcal{F}$ is the discrete Fourier transform operator. The intensity distribution at the detector is defined as $I(Z) = |F(Z)|^2$ (where the absolute value here is understood in the pointwise sense).

Beam stopping A beam stopping mask, or “beamstop”, is defined as $B \in \{0, 1\}^{2m \times 2n}$ such that it takes the value 0 in a region of low frequency and 1 everywhere else. The beam-stopped intensity image can then be written as $I(Z) \odot B$, where $\odot$ represents pointwise multiplication.

Measurement process Let $N_p > 0$ represent the expected mean number of photons incident per detector pixel. Then $(2m \times 2n)N_p$ is the expected total number of photons incident on the detector. The measurement data vector $Y \in \mathbb{R}^{2m \times 2n}$ is set to

$$Y \sim \frac{C}{N_p} \text{Poisson} \left( \frac{N_p}{C} I(Z) \odot B \right).$$

The constant $C$ is equal to the sum of all square Fourier magnitudes over the detector. The inner normalization constant $N_p/C$ ensures that the simulated setting corresponds on average to the measurement of $N_p$ expected photons per pixel. The outer normalization constant is applied to make $Y$ be of the same order of magnitude as $I(Z) \odot B$.

Holography setup We structure $Z$ into an unknown object $X$, and a known reference $R$. The setting we will use throughout this paper is as follows (see also Figure 2). Let $X, R \in \mathbb{R}^{m \times m}$, and set $X_0 = (X|0_{m \times m}|0_{m \times m}), R_0 = (0_{m \times m}|0_{m \times m}|R)$ with $X_0, R_0 \in \mathbb{R}^{m \times 3m}$. Then $Z = X_0 + R_0 = (X|0_{m \times m}|R)$. The region of zeros $0_{n \times m}$ separating object and reference represents the holographic separation condition. It is not necessary for our proposed methods (see Section 4.3), but required for several baseline methods. Thus to ensure a fair comparison, the separation setting will be our standard setting.

3. A reconstruction strategy adapted to low-photon CDI

We propose to maximize the likelihood of the measurements $Y$ given the underlying image $X$ and the CDI model above. This objective involves the likelihood of the Poisson-distributed measurements, accounting for the nature of noise in the low-photon regime, as well as the full forward model (including reference and beamstop): $X = \arg \max_X \log p(Y|X, N_p)$, where the distribution of $Y$ conditional on $X$ is given by Equation 2. Replacing the expression of the Poisson distribution
Figure 3: Comparing reconstructions across algorithms and noise levels on a sample image from SET12 (CAMERA, top) and a sample image from BIO10 (VIRUS, bottom) with a binary random reference and without beamstop. Figure 13 is a replicate for samples from COIL100. Corresponding SSIM scores can be found in Figure 4.
and dropping constants yields
\[
\hat{X} = \arg \max_X \sum_{ij(B)_{ij}=1} Y_{ij} \log I((X|0_{m \times m}|R))_{ij} - I((X|0_{m \times m}|R))_{ij}.
\]  
(3)

where the sum is taken only over non-zero entries of the beamstop mask. The optimization of this objective is performed directly using gradient ascent in PyTorch.

We investigate two strategies. The optimization is done either directly on the pixels of \( X \), as in Equation 3, or on the parameters of a deep decoder neural network prior encoding \( X \) (Heckel and Hand, 2019). We refer to these two variants as HolOpt-P for holographic Poisson likelihood optimization, and HolOpt-P-DD for holographic Poisson likelihood optimization with a deep decoder.

The deep decoder belongs to the class of untrained image priors: neural networks with image-shaped outputs trained by gradient descent to output one single image. The architecture of the network imposes an inductive bias favoring natural image statistics.

To formally describe HolOpt-P-DD, we denote by \( \sigma(\vartheta, z) \) the output of the deep decoder, where \( z \) corresponds to a fixed latent image and \( \vartheta = (\vartheta_1, \cdots, \vartheta_d) \) represents all the parameters \( \vartheta_i \) of the convolutional layers of a deep decoder of depth \( d \). We review the architecture of these networks in more detail in Appendix A. For HolOpt-P-DD, we set \( X = \sigma(\vartheta, z) \) and train all \( \vartheta_i \) in \( \vartheta \). In this second case the objective can be re-written as
\[
\hat{\vartheta} = \arg \max_{\vartheta} \sum_{ij(B)_{ij}=1} Y_{ij} \log I((\sigma(\vartheta, z)|0_{m \times m}|R))_{ij} - I((\sigma(\vartheta, z)|0_{m \times m}|R))_{ij}.
\]  
(4)

The reconstructed image is then the output of the deep decoder \( \hat{X} = \sigma(\hat{\vartheta}, z) \) after training on a single magnitude image \( Y \).

4. Experiments

Data Our strategy is demonstrated on the following datasets. SET12 is a dataset consisting of 12 images used as a traditional benchmark in image processing, here resized to 128 \times 128 pixels, while BIO10 , resized to 256 \times 256 pixels, contains 10 more realistic biological samples (these two...
datasets are available with the paper code). We also consider the COIL100 dataset (Nene et al., 1996) which contains 100 objects on a black background with $128 \times 128$ pixels. We explicitly zero out the background such that the support of the objects is not perfectly known. In contrast to non-holographic phase retrieval, a good reference should disambiguate the position of the sample within the frame. Hence, COIL100 allows us to test the robustness of the different algorithms to reference design. All images are converted to gray scale, and examples are presented in Figure 12 of the Appendix.

**Benchmark setup** The strategy proposed in this work is compared against three algorithms for holographic CDI: inverse filtering, Wiener filtering and Hybrid Input-Output modified for holographic phase retrieval, here referred to as HIO-Holo. We further augment HIO-Holo by selecting the best residual reconstruction over all iterations, to give it the fairest possible chance in our comparison. As discussed in Section 1.2, there is no comparable machine learning method that can be used here as a benchmark. However, we test variants of HolOpt-P and HolOpt-P-DD, termed HolOpt-S and HolOpt-S-DD respectively, in which mean squared error (MSE) is optimized instead of the Poisson likelihood. At high photon counts (low noise), Poisson noise is well-approximated by Gaussian noise and the two objectives are expected to perform similarly. However, their difference becomes significant at lower photon counts (high noise). The benefits of taking into account the Poisson nature of the noise are shown in experiments below.

**Hyperparameters** We use the Adam optimizer (Kingma and Ba, 2015) and learning rates varying between 0.01 and 0.1, depending on the loss and prior. For deep decoders, we observe the number of channels to only marginally change the outcome of the reconstruction, while varying the depth of the prior trades off precision of the reconstructed edges and finer details (shallower) with spatial regularity (deeper). The depth hyperparameter needs to be adjusted to the type of image analyzed and the noise level. In order to avoid overfitting, we select it for the first image of each dataset, and fix this value for the whole dataset. For optimal settings (Table 1) and a visualization of the effect of depth (Figure 11), see Appendix A.2. Practitioners are encouraged to tune the hyperparameters by visual inspection on one of their specimens, preferably the one for which they have the strongest prior knowledge, and leave these parameters fixed for all subsequent specimens.

**Evaluation** Algorithms are compared in terms of Structural Similarity Index (SSIM) Wang et al. (2004). Comparisons in terms of relative reconstruction error — Euclidean distance between the reconstructed $\hat{X}$ and ground truth specimen $X$ normalized by the $\ell_2$-norm of $X$ — and relative residual error — understood as the Euclidean distance between the observations $Y$ and the noiseless output of the forward model for a specimen $\hat{X}$ normalized by the $\ell_2$-norm of $Y$ — are also reported in the Appendix. Errors are averaged over images of each dataset as well as a few different random seeds for BIO10 and SET12 to increase the statistics of the small datasets. Error bars correspond to standard deviations.

### 4.1. Noisy reconstruction with and without the deep decoder

In a first series of experiments, we examine the robustness to noise of HolOpt-P and HolOpt-P-DD. We set the reference $R$ to a $m \times m$ binary array with entries 0 or 1 sampled uniformly and independently, a reference design generally very favorable to the reconstruction (Candès et al., 2015; Marchesini et al., 2008). No beamstop mask is included.

Figure 3 shows a clear qualitative improvement of our methods over the baselines as noise increases (observed consistently over the different datasets, see also Figure 13 in the Appendix).
Figure 5: An example reconstructed image from each of the SET12, BIO10, and COIL datasets, respectively, as a function of beamstop area fraction $a$ for fixed photon count $N_p = 1$. 
In Figure 4, HolOpt-P-DD consistently reaches higher SSIM scores in the noise range $N_p = 1$ to $N_p = 100$ across datasets. At very low noise $N_p = 1000$, the ordering of the methods varies, yet visual inspection confirms that all algorithms perform similarly and well, except for HolOpt-S-DD combining squared loss and deep decoder (see discussion below). On the other hand, at $N_p = 0.1$, little information is left for the algorithms to retrieve: all methods reconstruct images with SSIM scores close to 0.1, visually failing in different ways.

Among the variants of the proposed HolOpt, we observe the following trends. The reconstruction loss and visual quality of the samples are in almost all cases better with HolOpt-P than with HolOpt-S, validating our adoption of the most realistic noise model and Poisson likelihood objective. The difference between MSE and Poisson likelihood objectives is most drastic when including the deep decoder prior. In particular, the MSE loss sometimes leads to artifacts in the images reconstructed by HolOpt-S-DD (see Figures 3 and 13 in Appendix B). Thus, we focus only on the Poisson likelihood objective going forward. Regarding the use of a deep decoder, we distinguish several performance regimes for our method. At low noise ($N_p \approx 1000$ to 100), there is no need for regularization by a deep decoder, and HolOpt-P-DD achieves reconstructions of similar quality to HolOpt-P. Here, the SSIM is typically slightly worse with a deep decoder than without (except for COIL images). Including a prior is not harmful, but often unnecessary. At higher levels of noise, the denoising power of the deep decoder is beneficial. These observations are in accordance with the intuition that a prior helps when information is scarce, but is less helpful when observations of high quality are available.

4.2. Reconstructing with missing low frequencies

As discussed in Section 2, a universal feature of CDI experiments is a beamstop which obscures low-frequency magnitudes. In Wiener and inverse filtering, one simply sets the missing magnitudes to zero (Guizar-Sicairos and Fienup, 2007), whereas HIO-Holo can be made agnostic to the missing magnitudes. We show here that our optimization-based methods can effectively incorporate an arbitrary beamstop in the forward model, as defined in Equation 3. Moreover, we expect and indeed observe that the deep decoder prior can be particularly useful in compensating for the missing magnitudes.

We evaluate our methods HolOpt-P and HolOpt-P-DD at several noise levels and beamstop sizes, example reconstructions for SET12 and SSIMs plots for all datasets and in Figures 5 and 6 respectively. Supplemental plots for all datasets and noise levels are available in Figures 17-27 of the Appendix, including mean-squared error, which corroborate the trends observed here. We consider square beamstop masks centered at the 0 frequency, identified by their area fraction $a$: the fraction of the total measured magnitudes which are lost (visualized in Figure 17 of the Appendix).

We find that both HolOpt-P and HolOpt-P-DD vastly outperform HIO-Holo, Wiener and inverse filtering at near-all noise levels, test images, and beamstop area fractions. The advantage in terms of SSIM of the deep decoder prior is image-dependent: HolOpt-P-DD yields most significantly improved SSIM relative to HolOpt-P on BIO10 at low photon counts, and at all noise levels for COIL100, but makes little difference in SSIM on the SET12 dataset (see Figure 6). Yet visually, as in Figure 5, the reconstructions via HolOpt-P-DD on all datasets have enhanced contrast and details relative to HolOpt-P; furthermore, both HolOpt-P and HolOpt-P-DD visually outperform baselines. We note that even at settings where baselines achieve higher SSIM, notably with largest beamstop size and low photon counts on the COIL100 dataset, visual inspection of Figures 5 and
Figure 6: Reconstruction SSIM as a function of beamstop area fraction. Baseline methods are run for 5 trials per image across all datasets, while for tractability our methods are run for 2 trials each on BIO10 and SET12, and 1 trial each on COIL100. Average SSIM and one standard deviation error bars are shown. correspond to no missing data, i.e. formally $a = 0$ at the leftmost points.
22 illustrate that no method performs recognizable reconstruction at this beamstop size; the supposed improvement thus appears to be an idiosyncrasy of the SSIM. In sum, the performances of our methods smoothly degrade with increasing fraction of missing magnitudes α, and enable reconstructions with lower error (Figure 6) and visually improved features (Figure 5) relative to baselines. This provides powerful evidence that our method can enable refined reconstructions given even large fractions of lost magnitude data at the highest noise levels.

4.3. Robustness to reference separation

The separation distance between the specimen and the reference limits the smallest resolution that can be achieved (Salditt et al., 2020), and thus would ideally be minimized. For a specimen of size \( m \times m \) pixels, the holographic separation condition dictates that inverse filtering and Wiener filtering require a full separation \((X|0_{m \times m}, R)\). In contrast, our approach only requires that the forward model be differentiable, which is the case for any reference placement.

Here, we explore signal-reference association of the form \((X|R|0_{m \times m})\), where \( R \) is a random binary block of small size: it is non-zero only on a box of size \(0.1m \times 0.1m\) with uniformly and independently chosen entries in \(\{0, 1\}\), and the box position is varied between experiments. No beamstop is included. Figure 7 displays example reconstructions for \(N_p = 10\) and \(N_p = 1\) and Figure 8 reports achieved SSIM scores as a function of the relative specimen-reference separation for the three datasets and multiple levels of noises. The only applicable baseline is HIO-Holo, illustrating the challenging nature of this setting.

For the three compared methods, the quality of the reconstruction depends slightly on the separation, only HIO-Holo at 0 separation generates clearly poorer images. Visually, HIO-Holo yields the less sharp images and HolOpt-P-DD is almost always the best algorithm. Without the deep decoder, HolOpt-P reconstructions are also of good quality but sometimes show less contrast. The neural network prior makes a difference in particular at high levels of noise and on COIL100 images, for which the deep decoder captures well the solid black background. These observations are consistent with the average SSIM, but we note that the variance across images in the dataset can be significant. At very high noise \(N_p = 0.1\) photon/pixel, HIO-Holo has better SSIM scores than HolOpt-P methods, yet this is arguably the limit of reconstruction possibilities for any of the methods (SSIM < 0.2 and visuals in Figure 15).

Overall, this more challenging experimental setting confirms the efficiency of our proposed method, allowing reconstruction even if the holographic separation condition is broken. Moreover, a deep decoder prior provides clear benefits even over direct optimization in certain cases.

4.4. Varying the oversampling rate

In a last experiment, we consider yet another challenge for reconstruction by lowering the oversampling rate of the observation. For oversampling factors larger or equal to 2, the inverse problem can be solved exactly in the absence of noise (Hayes, 1982). In the presence of noise, increased oversampling is all the more beneficial, as collecting more information can compensate for the noise corruption. We test how our methods perform relative to HIO-Holo for oversampling ratios around

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2. We note that the performance of Wiener and inverse filtering suffers at small beamstop sizes due to the “ringing” effect of low frequencies, an effect which occurs regardless of the method for filling the low magnitudes. Evident as a striping effect in Figure 5, this explains the occasional increase in SSIM with increasing beamstop size evident in Figure 6.
Figure 7: Reconstruction errors for photon counts $N_p = 10$ (left) and $N_p = 1$ (right) with a $0.1m \times 0.1m$ binary random reference as a function of the relative separation. A separation of 0.5 implies that the left-most non-zero pixel of the reference is 0.5 pixels away form the image. See Figure 15 in Appendix for $N_p = 100$ and $N_p = 0.1$. 
Figure 8: Reconstruction SSIM for decreasing photon counts $N_p$ as a function of the relative separation (see caption of Figure 7). Corresponding MSEs are plotted in Figure 16 of the Appendix.

Figure 9: Reconstructed images for samples from SET12, BIO10 and COIL100 datasets with varying oversampling factors (numbers above each column) at $N_p = 10$ photon/pixel.
Figure 10: Average SSIM scores for SET12, BIO10 and COIL100 with varying oversampling factor at $N_p = 10$ photon/pixel. Errors bars represent standard deviations.

the critical value of 2. Note that inverse and Wiener filtering are not well-defined for oversampling rates smaller than 2. Figures 9 and 10 display results for a well-separated binary reference and without beamstop at $N_p = 10$ photon/pixel (see Appendix B.4 for identical figures at $N_p = 1$). All images reconstructed by HolOpt-P-DD are visually superior to images reconstructed by HIO-Holo at oversampling factors both smaller and larger than 2. HolOpt-P-DD also produces sharper images than HIO-Holo, although sometimes with less contrast. This phenomenology is largely captured by the SSIM.

5. Discussion and Conclusion

In this paper, we have shown that recent progress at the intersection of machine learning and inverse problems can yield highly successful algorithms which also account for realistic experimental challenges. Our novel optimization framework for holographic phase retrieval improves on state-of-the-art reconstruction, even in the most difficult experimental settings and without external training data. Untrained image priors are confirmed to be powerful tools, especially when a significant amount of information is missing from the measured data due to low photon counts, beamstop-obscured frequencies and small oversampling. Due to its practicality and flexibility, we believe our methodology should prove valuable for practitioners. While this work demonstrated our approach’s success on simulated observations, we expect to confirm its findings on experimental data in future work. Finally, our framework is easily adaptable to different variants of the problem — even the mathematically distinct non-holographic setting — and should enable similarly improved reconstruction with other imaging modalities than Holographic CDI, such as optical holography (He et al., 2015), magnetic holographic imaging (Hu et al., 2019), and ptychography (Wen et al., 2012).

ACKNOWLEDGMENTS

The authors would like to thank Charlie Epstein, Leslie Greengard and Alex Barnett for insightful discussions. D.B acknowledges Ju Sun and Emmanuel Candès for helpful suggestions and discussions on the development of these methods and ideas. H. L. is supported by the Fannie and John Hertz Foundation.
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Figure 11: Impact of depth of a deep decoder prior on the reconstruction illustrated on VIRUS. Left: Relative residual errors and reconstruction errors as a function of depth. Right: Best reconstruction out of 10 runs.

Appendix A. The deep decoder

In this section we provide further information regarding the deep decoder prior.

A.1. Deep decoder architecture

The deep decoder essentially consists of an alternation of two operations — convolutions with filter size of $1 \times 1$ pixels, and upsampling by a factor of 2 using bilinear interpolation. The input is a randomly initialized image of smaller size. In order to end up with a specific output image size, either the input image size or the number of layers $d$ is adjusted.

Let $c_i$ represent the number of channels at layer $i$ and let $\vartheta_i \in \mathbb{R}^{c_i+1 \times c_i \times 1 \times 1}$ represent the convolution kernels at layer $i$. Denote by $\text{conv}_{\vartheta_i}$ the typical deep learning convolution with $\vartheta_i$, by $\text{up}_2$ the bilinear upsampling operation, and by $\text{relu}(x) = x_{x > 0}$.

Then we can define one component as

$$\text{block}_i := \text{up}_2 \circ \text{relu} \circ \text{conv}_{\vartheta_i}$$

and the full network as

$$\text{net} := \text{block}_d \circ \cdots \circ \text{block}_1.$$ 

For an input image $z \in \mathbb{R}^{1 \times c_1 \times \kappa \times \lambda}$, let

$$\sigma(\vartheta, z) = \sigma(\vartheta_d, \ldots, \vartheta_1, z) = \text{net}(z),$$

where $\vartheta = (\vartheta_d, \ldots, \vartheta_1)$ collects all the convolution parameters. In our experiments we set $\mathbf{X} = \sigma(\vartheta, z)$ and train the parameters $\vartheta_i$.

A.2. Selection of depth and number of channels

When using a deep decoder to reconstruct one needs to specify the number of channels of its convolutional filters, as well as the number of layers. Across images and noise levels, we observed that the performance is marginally affected by the number of channels, except for the fact that it deteriorates for number of channels below a certain threshold (around 64 for our examples). To fine-tune a specific reconstruction it can be useful to adjust this parameter, e.g. to limit the fitting power of the
Table 1: Depth, number of channels, and number of optimizer steps used for the deep decoder in all experiments.

| Noise       | \( N_p = 1000 \) | \( N_p = 100 \) | \( N_p = 10 \) | \( N_p = 1 \) | \( N_p = 0.1 \) |
|-------------|------------------|----------------|----------------|----------------|----------------|
| SET 12      | d2 c128          | d3 c128        | d2 c128        | d1 c128        | d1 c128        |
| COIL100     | d2 c128          | d2 c128        | d2 c128        | d1 c128        | d1 c128        |
| BIO10       | d3 c128          | d3 c128        | d2 c128        | d2 c128        | d2 c128        |
| # iterations| 10000            | 10000          | 5000           | 2500           | 1250           |

model at high noise levels, as pointed out by Hand et al. (2018), yet its impact is much more subtle than that of depth.

In Figure 11, we illustrate this fact by reporting errors and reconstructed images of first BIO10 image (VIRUS) as a function of depth for different noise levels. Visually, deeper decoders render smoother images. This is a direct consequence of the upsampling layers which correlates the neighboring pixels. The deeper the decoder, the smaller the latent representation \( z \) and the less independent the output pixels. Note that at high noise levels (\( N_p = 1 \)) the smoothing reduces the reconstruction error estimated using Euclidean distance. Perceptually however, the smoothing is only beneficial to some extent. Note that while the sum of errors across pixels is greater for shallow models, large mistakes are more evenly distributed whereas for the deep models they are concentrated on edges of the object in the picture. Our eyes are found to be excellent denoisers for speckles. At lower noise levels (\( N_p = 10 \)), the excess of depth can be spotted directly in the reconstruction error as we observe a dip in the curve.

Following these observations, we select the parameters of the deep decoders used in our experiments according to the best visual outcomes on the first image of each dataset for each level of noise. The selected parameters, gathered in Table 1, are then employed for all the images of the given dataset. Table 1 also includes number of steps in the gradient descent. Some early stopping was found beneficial in order to avoid overfitting at high noise levels. As a result we adapt the number of iterations to the photon count.

Appendix B. Additional figures

In this section we provide additional figures for experiments presented in the main text. Figure 12 display sample images of the three datasets used for experiments.

B.1. Noisy reconstruction experiment

Figures 13 and 14 present results for the experiment described in 4.1 of the main text. The superior visual quality of our algorithms is confirmed on samples form BIO10 and COIL100. In Figure 14 we compare methods in terms of residual \( \ell^2 \) error minimization and MSE. These measure appear less informative of the perceived similarity of ground truth and reconstructed images than SSIM. In particular, it should be observed that the residual error reflects performance neither perceptually nor according to the other error metrics.
B.2. Robustness to separation experiment

Figure 15, similar to 7, displays visual of the reconstruction as a function of the separation between sample and reference for two additional noise levels. In Figure 16 we report MSEs averaged over the datasets as a function of the separation. Observations on the ordering of the methods and dependence with separation are comparable with the observations drawn from SSIM plots in the main text.

B.3. Missing low-frequencies (beamstop) experiment

We now visualize the beamstop area fractions tested in Section 4.2 (see Figure 17), as well as show analogous plots to Figures 5 for all three test images and for all remaining noise levels, $N_p = 10, 100, 1000$ (Figures 19-27). Figure 18 also plots all settings using $\ell - 2$ errors.

B.4. Oversampling experiment

To complement results in the main text, Figure 28 displays reconstruction MSEs as a function of the oversampling rate as a function of the oversampling rate of the observations at $N_p = 10$. Figure 29 and Figure 30 focus on the noise level $N_p = 1$ photon / pixel and are similar to Figures already given at $N_p = 10$. 

Figure 12: Example images from datasets used in the experiments of this paper: SET12 (128x128 pixels), BIO10 (256x256 pixels) and COIL100 (128x128 pixels)
Figure 13: Comparing reconstructions across algorithms and noise levels on a sample of images from COIL100 with a binary random reference and without beamstop. Same as Figure 3.
Figure 14: Relative mean squared errors on the reconstructions and residual mean squared error averaged over the datasets. These are different metrics from the SSIM scores presented on Figure 4 to analyze the results of the experiment presented of Section 4.1.
Figure 15: Reconstructed images as a function of the relative separation as described in caption of Figure 16. Images correspond to the best of 10 runs in terms of residual error.
Figure 16: Reconstruction errors for decreasing photon counts $N_p$ with a $0.1m \times 0.1m$ binary random reference as a function of the relative separation. A separation of 0.5 implies that the left-most non-zero pixel of the reference is $0.5m$ pixels away from the image. Dashed lines corresponds to best run out of the 10 runs in terms of residual error.
Figure 17: Examples of the measured magnitudes corresponding to varying beamstop area fractions for the first image of SET12, CAMERA, with $N_p = 10$. 

\[ a = 0 \times 10^0 \]
\[ a = 5 \times 10^{-5} \]
\[ a = 1 \times 10^{-4} \]
\[ a = 5 \times 10^{-4} \]
\[ a = 1 \times 10^{-3} \]
\[ a = 5 \times 10^{-3} \]
\[ a = 1 \times 10^{-2} \]
\[ a = 5 \times 10^{-2} \]
\[ a = 1 \times 10^{-1} \]
Figure 18: Reconstruction errors on all three datasets (one per row, as indicated by the leftmost row levels) as a function of beamstop area fraction. Errors and error bars are computed as in Figure 4. The leftmost datapoints at $a = 1e-6$ correspond to no missing data, i.e. $a = 0$ at the leftmost points.
Figure 19: Reconstructed SET12 image with varying beamstop at $N_p = 10$ photons.

Figure 20: Reconstructed SET12 image with varying beamstop at $N_p = 100$ photons.
Figure 21: Reconstructed SET12 image with varying beamstop at $N_p = 1000$ photons.

Figure 22: Reconstructed COIL image with varying beamstop at $N_p = 10$ photons.
Figure 23: Reconstructed COIL image with varying beamstop at $N_p = 100$ photons.

Figure 24: Reconstructed COIL image with varying beamstop at $N_p = 1000$ photons.
Figure 25: Reconstructed BIO10 image with varying beamstop at $N_p = 10$ photons.

Figure 26: Reconstructed BIO10 image with varying beamstop at $N_p = 100$ photons.
Figure 27: Reconstructed BIO10 image with varying beamstop at $N_p = 1000$ photons.

Figure 28: Reconstruction $\ell^2$-errors for SET12, BIO10 and COIL100 with varying oversampling factor at $N_p = 10$ photon/pixel. Corresponding SSIM and visuals are displayed in Figures 10 and 9.
Figure 29: Reconstructed images for SET12, BIO10 and COIL100 with varying oversampling factors (numbers above each column) at $N_p = 1$ photon/pixel.

Figure 30: Reconstruction SSIM and $\ell_2$-errors for SET12, BIO10 and COIL100 with varying oversampling factor at $N_p = 1$ photon/pixel. Corresponding visuals are displayed in Figure 29.