
Phase Retrieval Using Double Deep Image Priors

Anonymous Author(s)

Affiliation

Address

email

Abstract

1 Phase retrieval (PR) concerns the recovery of complex phases from complex
2 magnitudes. We identify the connection between the difficulty level and the
3 number and variety of symmetries in PR problems. We focus on the most difficult
4 far-field PR (FFPR), and propose a novel method using double deep image priors.
5 In realistic evaluation, our method outperforms all competing methods by large
6 margins. As a single-instance method, our method requires no training data and
7 minimal hyperparameter tuning, and hence enjoys good practicality.

8 1 Introduction

9 In scientific imaging, observable physical quantities about the object of interest are often complex-
10 valued, e.g., when diffraction happens [1]. However, practical detectors can only record complex
11 magnitudes, but not phases, resulting in phaseless observations. Phase retrieval (PR), broadly defined,
12 is the nonlinear inverse problem of estimating the object of interest from the phaseless observations.
13 PR is central to coherent diffraction imaging ((B)CDI) [2, 3], image-based wavefront sensing [4],
14 radar and sonar sensing [5]; see the recent survey [6].

15 **Which phase retrieval (PR)?** Consider a 2D object of interest $\mathbf{X} \in \mathbb{C}^{m \times n}$, and a physical
16 observation model \mathcal{A} that leads to an ideal complex-valued observation $\mathcal{A}(\mathbf{X}) \in \mathbb{C}^{m' \times n'}$. However,
17 the detector can only record $\mathbf{Y} = |\mathcal{A}(\mathbf{X})|^2$, where $|\cdot|^2$ denotes the elementwise squared magnitudes.
18 **In far-field (Fraunhofer) PR (FFPR) that stems from far-field propagation and is also the focus**
19 **of this paper**, \mathcal{A} is the oversampled 2D Fourier transform \mathcal{F} with $m' \geq 2m - 1$ and $n' \geq 2n - 1$
20 to ensure recoverability. Numerous other \mathcal{A} 's have been studied in the literature, notable ones
21 including: **(1) Generalized PR (GPR)**: $\mathcal{A}(\mathbf{X}) = \{\langle \mathbf{A}_i, \mathbf{X} \rangle\}_{i=1}^k$ where \mathbf{A}_i 's are iid Gaussian
22 or randomly-masked Fourier basis matrices [7, 8]. These elegant mathematical models do not
23 correspond to physically feasible imaging systems so far; **(2) Near-Field (Fresnel) PR (NFPR)**:
24 $\mathcal{A}(\mathbf{X}) = \mathcal{F}(\mathbf{X} \odot [e^{i\pi\beta(i^2+j^2)}]_{i,j})$ [9, 10], where the constant $\beta > 0$ depends on the sampling
25 intervals, wavelength, and imaging distance [11], comes from near field propagation. Note that FFPR
26 corresponds to $\beta \rightarrow 0$, and PR problems solved in image-based wavefront sensing for astronomical
27 applications correspond to multi-plane near-field propagation with sequential optical aberrations [12];
28 **(3) Holographical PR (HPR)**: $\mathcal{A}(\mathbf{X}) = \mathcal{F}([\mathbf{X}, \mathbf{R}])$, where \mathbf{R} is a known reference that is put
29 side-by-side with the object of interest \mathbf{X} [13]; depending on the propagation distance, near-field
30 versions are also possible [1, Chapter 11]; **(4) Ptychography (PTY)**: \mathbf{X} is raster scanned by a sharp
31 illumination pattern \mathbf{W} that is focused over a local patch of \mathbf{X} each time. Now \mathbf{Y} is the set of
32 magnitude measurements $\mathbf{Y}_i = |\mathcal{F}(\mathbf{W} \odot \mathbf{X}(\mathbf{p}_i))|^2$, where \mathbf{p}_i indexes the raster grid [14, 15].

33 **Symmetry matters** Identifiability in PR is often up to intrinsic symmetries. For example, any
34 global phase factor $e^{i\theta}$ added to \mathbf{X} leaves \mathbf{Y} unchanged for FFPR, NFPR, GPR, and PTY, i.e.,
35 **global phase symmetry**. While this is the only symmetry for NFPR, GPR, and PTY, FFPR has

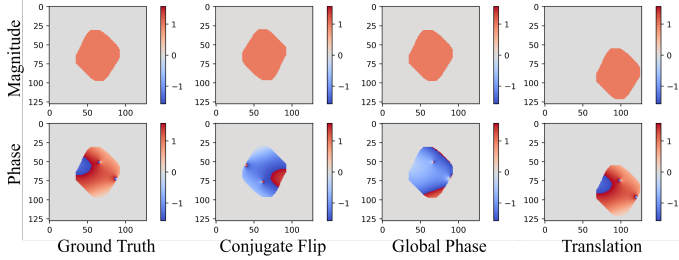


Figure 1: Illustration of the three intrinsic symmetries in FFPR on simulated complex-valued crystal data (see Section 4 for details). Any composition of 2D conjugate flipping, translation, and global phase, when applied to \mathbf{X} , leads to the same set of magnitudes \mathbf{Y} .

Table 1: Comparison of GPR, NFPR, and FFPR in terms of their symmetries and numerical solvability with the least-squares (LS) formulation combined with gradient descent.

PR model	GPR	NFPR	FFPR
Symmetry	global phase	global phase	global phase, translation, 2D conjugate flipping
Final loss of solving LS using gradient descent from 100 random initializations			

36 two other symmetries: translation and 2D conjugate flipping, as shown in Fig. 1 [16]. A crucial
 37 empirical observation is that **the difficulty level of a PR problem is proportional to the number**
 38 **of its symmetries**. To see the point, consider a natural least-squares (LS) formulation of PR:
 39 $\min_{\mathbf{X} \in \mathbb{C}^{m \times n}} \frac{1}{m'n'} \|\sqrt{\mathbf{Y}} - |\mathcal{A}(\mathbf{X})|\|_F^2$, with the groundtruth complex-valued 2D crystal sample in
 40 Fig. 1 as the target \mathbf{X} . On GPR with Gaussian, NFPR, and FFPR, we run gradient descent with 100
 41 random starts respectively and record their final convergent losses. As evident from Table 1, while we
 42 can consistently find numerically satisfactory solutions for GPR and NFPR, we always find bad local
 43 solutions for FFPR—which has three symmetries. Similarly, for FFPR, the gold-standard hybrid
 44 input-output (HIO) algorithm can typically solve the problem when provided with tight support
 45 specification—translation symmetry is killed, but HIO fails when the support is loose—translation
 46 symmetry remains; see Appendix A. Moreover, prior works [17–20] also show the learning difficulties
 47 caused by these symmetries when one develops data-driven methods for solving FFPR.

48 **Our focus on practical FFPR methods** We have stressed that symmetries largely determine
 49 the difficulty level of PR. However, in previous research, there are often simplifications to FFPR,
 50 including (1) **randomized the model** \mathcal{A} that only keeps the global phase symmetry, (2) **evaluation**
 51 **on natural images** that removes the translation symmetry and simplifies the global phase symmetry
 52 into sign symmetry [8, 21, 22]. These simplifications invariably lead to FFPR methods that do not
 53 work on practical data. **The goal of this paper is to develop practical methods for FFPR that**
 54 **involve all three symmetries**. In particular, we propose a novel FFPR method based on double deep
 55 image priors (see Section 3), and validate its superiority over state-of-the-art (SOTA) on realistic
 56 datasets (see Section 4).

57 2 FFPR: Formulation and Prior Arts

58 **FFPR model** The object of interest is $\mathbf{X} \in \mathbb{C}^{m \times n}$, and $\mathbf{Y} = |\mathcal{F}(\mathbf{X})|^2 \in \mathbb{R}_+^{m' \times n'}$. Here, \mathcal{F} is the
 59 oversampled 2D Fourier transform. We always assume that $m' \geq 2m - 1$ and $n' \geq 2n - 1$, which is
 60 necessary to ensure recoverability.

61 **Prior arts on FFPR** Since we focus on practical FFPR, here we only discuss methods that have
 62 been tested on FFPR with at least partial success. (I) **Classical iterative methods**: Due to the failure
 63 of the LS, most (if not all) classical methods tackle the over-parameterized feasibility reformulation:
 64 find $\mathbf{Z} \in \mathbb{C}^{m' \times n'}$ s. t. $|\mathcal{F}(\mathbf{Z})|^2 = \mathbf{Y}$, $\mathcal{L}(\mathbf{Z}) = \mathbf{0}$, where \mathcal{L} restricts \mathbf{Z} to the zero-padding locations
 65 defined by the oversampling. **More refined support information can be naturally incorporated**

66 **into the support constraint** $\mathcal{L}(\mathbf{Z}) = \mathbf{0}$. These classical methods are all based on generalized
67 alternating projection, represented by error-reduction (ER), hybrid input-output (HIO) [23], reflection
68 average alternating reflectors (RAAR) [24], difference map (DM) [25], and oversampling smoothness
69 (OSS) [26]. They are empirically observed to find good solutions for FFPR, provided that the support
70 specification for \mathbf{Z} is tight and hyperparameters are properly tuned. Alternative formulations solved
71 by second-order methods [27, 28] are less sensitive to hyperparameters. However, all these methods
72 require tight support specification to avoid the translation symmetry—failing so leads to spurious
73 solutions that look like the superposition of translated copies; see Appendix B. This is addressed
74 by the popular **shrinkwrap** trick [29] in practice, which refines the support by smoothing-and-
75 thresholding over iterations. **(II) Data-driven methods: The first line of work** represents the inverse
76 mapping from \mathbf{Y} to \mathbf{X} by a deep neural network (DNN) g_θ , which is trained either over an extensive
77 training set $\{(\mathbf{Y}_i, \mathbf{X}_i)\}_i$, or unpaired $\{\mathbf{Y}_i\}_i$ and $\{\mathbf{X}_i\}_i$ only by observing the cycle consistency
78 constraint: $|\mathcal{F}(g_\theta(\mathbf{Y}))|^2 \approx \mathbf{Y}$ [30–35, 17–20, 36, 37]. But, as discussed in [17–20], symmetries in
79 the problem cause substantial learning difficulties, as any \mathbf{Y} maps to a family of equivalent \mathbf{X} ’s.
80 **The second line of work** [38–40] is tied to specific iterative methods for solving FFPR and replaces
81 certain components of these methods with trainable DNNs. A common limitation of this line is the
82 reliance on good initialization that is obtained from classical iterative methods. Therefore, this family
83 can be viewed as a final refinement of the results from classical methods and does not address the
84 essential difficulty of solving FFPR. **Both lines** suffer in generalization when the training data are not
85 sufficiently representative.

86 Our method overcomes the limitations of both classical and data-driven methods. (1) **No training set:**
87 it works with a single problem instance each time, with zero extra training data; (2) **No shrinkwrap:**
88 we can specify the size of \mathbf{X} directly as $\lfloor m'/2 \rfloor \times \lfloor n'/2 \rfloor$, i.e., the information-theoretic recovery
89 limit, without worrying about the translation symmetry; (3) **Minimal tuning:** mostly we only need to
90 tune 2 learning rates as hyperparameters, vs. the 5 or 6 hyperparameters used in HIO+ER+Shrinkwrap
91 (HES) for practical CDI [41].

92 3 Our method: FFPR using double DIPs

93 **Deep image prior (DIP) for visual inverse problems** DIP and variants [42] parameterize visual
94 objects as outputs of DNNs—typically structured convolutional networks to favor spatially smooth
95 structures, i.e., $\mathbf{x} = G_\theta(\mathbf{z})$, where \mathbf{z} is normally a random but fixed seed, and G_θ is a trainable DNN
96 parameterized by θ . For a visual inverse problem of the form $\mathbf{y} \approx f(\mathbf{x})$ where \mathbf{y} is the observation
97 and f is the observation model, the classical regularized data-fitting formulation $\min_{\mathbf{x}} \ell(\mathbf{y}, f(\mathbf{x})) +$
98 $\lambda\Omega(\mathbf{x})$ can now be empowered by DIP and turned into $\min_{\theta} \ell(\mathbf{y}, f \circ G_\theta(\mathbf{z})) + \lambda\Omega \circ G_\theta(\mathbf{z})$. This
99 simple idea has recently claimed numerous successes in computer vision and imaging; see, e.g.,
100 [43–46]. **A salient feature of DIP is the strong structured prior it imposes through DNNs, with**
101 **zero extra data!** Although the theoretical understanding of DIP is still far from complete, current
102 theories attribute its success to two aspects: (1) **structured priors** imposed by convolutional and
103 upsampling operations, and (2) **global optimization** due to significant overparameterization and
104 first-order methods [47, 48].

105 **Applying DIP to FFPR** As shown in Table 1, solving the LS formulation using gradient descent
106 always gets trapped in bad local minimizers. It is then tempting to try DIP, as (1) the objects we try to
107 recover in scientific imaging are visual objects and probably can be blessed by the structured priors
108 enforced by DIP, and (2) more importantly, the issue we encounter in solving the LS is exactly about
109 global optimization, which could be eliminated by overparameterization in DIP. In fact, systematic
110 evaluation of solving $\min_{\theta} \|\sqrt{\mathbf{Y}} - |\mathcal{F} \circ G_\theta(\mathbf{z})|\|_{\mathcal{F}}^2$ where $G_\theta(\mathbf{z}) \in \mathbb{C}^{m \times n}$ in Figs. 2 and 3 shows
111 that it is already competitive compared to the gold-standard HES, although it struggles to reconstruct
112 complicated complex phases.

113 **Double DIPs boost the performance** For FFPR applications such as CDI, \mathbf{X} as a complex-valued
114 object can often be naturally split into two parts with disparate complexity levels. For example, in
115 Bragg CDI on crystals, the magnitude part on the support is known to have uniform values, but
116 the phase part can have complex spatial patterns due to strains [49–51]; in CDI on live cells, the
117 nonnegative real part contains useful information, and the imaginary part acts like small-magnitude
118 noise [52]. In these cases, due to the apparent asymmetry in complexity, it makes sense to parameterize

119 X as two separate DIPs [53, 46] instead of one:

$$X = G_{\theta_1}^1(z_1)e^{iG_{\theta_2}^2(z_2)}, \text{ or } X = G_{\theta_1}^1(z_1) + iG_{\theta_2}^2(z_2). \quad (1)$$

120 This can be justified as balancing the learning paces: with a single DIP, “simple” part is learned
 121 much faster than the “complex” part; with double DIPs, we can balance the learning paces by making
 122 the learning rate for the “simple” part relatively small compared to that for the “complex” part. So
 123 we observe a substantial performance boost in Figs. 2 and 3 due to the double-DIP parametrization.

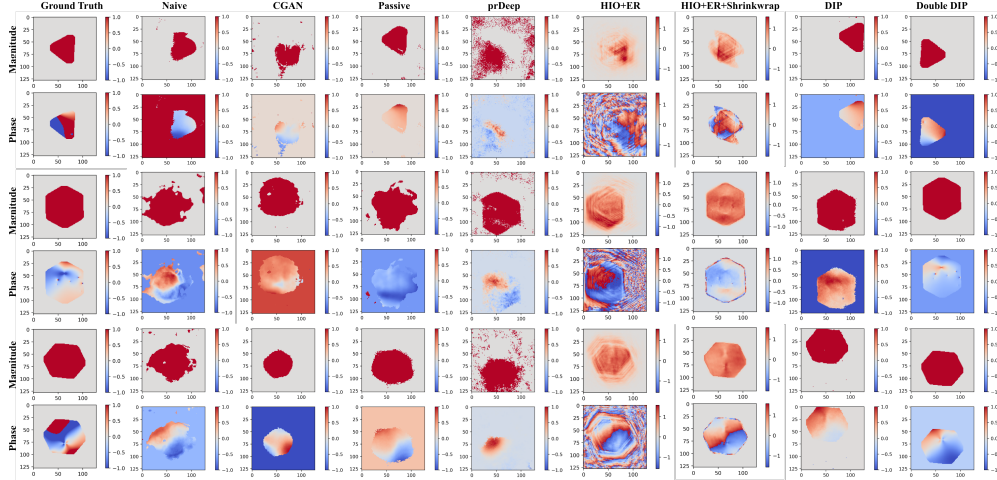


Figure 2: Visual comparison of reconstruction results by different methods on 2D crystal data

124 4 Experiments Results

125 We first compare our Double-DIP method
 126 with multiple SOTA methods for FFPR, including Naive [36], CGAN [54], Passive [32],
 127 prDeep [38], HIO+ER, HIO+ER+Shrinkwrap (HES), and (single-)DIP on simulated 2D data
 128 for Bragg CDI on crystals. The final form of our learning objective for this task is:
 129
 130
 131

$$\min_{\theta_1, \theta_2} \|\sqrt{Y} - |\mathcal{F} \circ G_{\theta_1}^1(z_1)e^{iG_{\theta_2}^2(z_2)}|\|_{F}^2. \quad (2)$$

132 To ensure that the evaluation data reflect real-world complexity, we simulate 2D complex-
 133 valued crystal data in Bragg CDI applica-
 134 tions [3]. The dataset is generated by first creating 2D convex and nonconvex shapes based on
 135 random scattering points in a 110×110 grid on a 128×128 background. The complex magnitudes
 136 are uniformly 1, and the complex phases are determined by projecting the simulated 2D displacement
 137 fields (due to crystal defects) onto the corresponding momentum transfer vectors. To maximize
 138 the diversity, the dataset contains diverse shapes and different numbers and densities of crystal
 139 defects that directly determine the complexity of the phases. **Although our double-DIP method is a**
 140 **single-instance method that requires no training data, the dataset is large enough to support**
 141 **data-driven methods, such as Passive and prDeep.** For methods that require a training set, we
 142 provide 8000 samples. All methods are tested on 50 samples. From both visual (Fig. 2) and quantitative (Fig. 3) results, it is evident that: (1) all data-driven methods, including Naive, CGAN, Passive, prDeep, perform poorly. We believe that this is due to either the learning difficulty caused by the three symmetries [17–20] or the bad initialization given by HIO (i.e., for prDeep); (2) HES, DIP, and our double-DIP are the top three methods. HES deals with translation symmetry by explicitly iterative refining the support, whereas DIP and ours do not need tight support estimation at all, substantially reducing parameter tuning; (3) Our method wins HES and DIP by a large margin. Although the latter two perform reasonably well in magnitude estimation, their phase estimations are typically off for complicated instances. Appendix C contains evaluation on 3D simulated Bragg CDI data.
 143
 144
 145
 146
 147
 148
 149
 150
 151

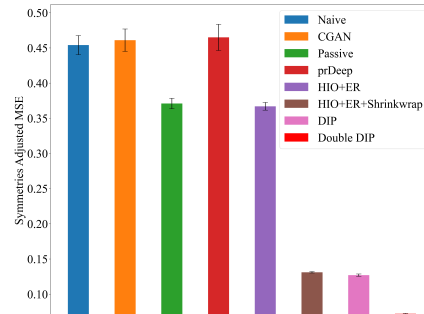


Figure 3: Quantitative comparison of reconstruction results by different methods on 2D simulated crystal data by symmetry-adjusted MSE

References

- 152 [1] Joseph W. Goodman, *Introduction to Fourier Optics*, Freeman & Company, W. H., 4th edition, 2017.
- 153 [2] Jianwei Miao, Pambos Charalambous, Janos Kirz, and David Sayre, "Extending the methodology of x-ray
154 crystallography to allow imaging of micrometre-sized non-crystalline specimens," *Nature*, vol. 400, no.
155 6742, pp. 342–344, 1999.
- 156 [3] I. K. Robinson, I. A. Vartanyants, G. J. Williams, M. A. Pfeifer, and J. A. Pitney, "Reconstruction of the
157 shapes of gold nanocrystals using coherent x-ray diffraction," *Physical Review Letters*, vol. 87, no. 19, pp.
158 195505, oct 2001.
- 159 [4] D. Russell Luke, James V. Burke, and Richard G. Lyon, "Optical wavefront reconstruction: Theory and
160 numerical methods," *SIAM Review*, vol. 44, no. 2, pp. 169–224, jan 2002.
- 161 [5] Philippe Jaming, "Phase retrieval techniques for radar ambiguity problems," *The Journal of Fourier
162 Analysis and Applications*, vol. 5, no. 4, pp. 309–329, jul 1999.
- 163 [6] Yoav Shechtman, Yonina C. Eldar, Oren Cohen, Henry Nicholas Chapman, Jianwei Miao, and Mordechai
164 Segev, "Phase retrieval with application to optical imaging: A contemporary overview," *IEEE Signal
165 Processing Magazine*, vol. 32, no. 3, pp. 87–109, may 2015.
- 166 [7] Emmanuel J Candes, Yonina C Eldar, Thomas Strohmer, and Vladislav Voroninski, "Phase retrieval via
167 matrix completion," *SIAM review*, vol. 57, no. 2, pp. 225–251, 2015.
- 168 [8] Albert Fannjiang and Thomas Strohmer, "The numerics of phase retrieval," *Acta Numerica*, vol. 29, pp.
169 125–228, may 2020.
- 170 [9] Fei Wang, Yaoming Bian, Haichao Wang, Meng Lyu, Giancarlo Pedrini, Wolfgang Osten, George Barbas-
171 tathis, and Guohai Situ, "Phase imaging with an untrained neural network," *Light: Science & Applications*,
172 vol. 9, no. 1, may 2020.
- 173 [10] Yuhe Zhang, Mike Andreas Noack, Patrik Vagovic, Kamel Fezzaa, Francisco Garcia-Moreno, Tobias
174 Ritschel, and Pablo Villanueva-Perez, "PhaseGAN: a deep-learning phase-retrieval approach for unpaired
175 datasets," *Optics Express*, vol. 29, no. 13, pp. 19593, jun 2021.
- 176 [11] Tomoyoshi Shimobaba and Tomoyoshi Ito, *Computer Holography Acceleration Algorithms and Hardware
177 Implementations*, Taylor & Francis Group, 2019.
- 178 [12] J. R. Fienup, "Phase-retrieval algorithms for a complicated optical system," *Applied Optics*, vol. 32, no.
179 10, pp. 1737, apr 1993.
- 180 [13] David A. Barmherzig and Ju Sun, "Towards practical holographic coherent diffraction imaging via
181 maximum likelihood estimation," *Optics Express*, vol. 30, no. 5, pp. 6886, feb 2022.
- 182 [14] Pierre Thibault, Martin Dierolf, Andreas Menzel, Oliver Bunk, Christian David, and Franz Pfeiffer,
183 "High-resolution scanning x-ray diffraction microscopy," *Science*, vol. 321, no. 5887, pp. 379–382, jul
184 2008.
- 185 [15] Stefano Marchesini, Andre Schirotzek, Chao Yang, Hau tieng Wu, and Filipe Maia, "Augmented projections
186 for ptychographic imaging," *Inverse Problems*, vol. 29, no. 11, pp. 115009, oct 2013.
- 187 [16] Tamir Bendory, Robert Beinert, and Yonina C. Eldar, "Fourier phase retrieval: Uniqueness and algorithms,"
188 in *Compressed Sensing and its Applications*, pp. 55–91. Springer International Publishing, 2017.
- 189 [17] Kshitij Tayal, Chieh-Hsin Lai, Vipin Kumar, and Ju Sun, "Inverse problems, deep learning, and symmetry
190 breaking," *arXiv:2003.09077*, Mar. 2020.
- 191 [18] Raunak Manekar, Kshitij Tayal, Zhong Zhuang, Chieh-Hsin Lai, Vipin Kumar, and Ju Sun, "Breaking
192 symmetries in data-driven phase retrieval," in *OSA Imaging and Applied Optics Congress 2021 (3D, COSI,
193 DH, ISA, pcAOP)*. 2021, Optica Publishing Group.
- 194 [19] Kshitij Tayal, Chieh-Hsin Lai, Raunak Manekar, Zhong Zhuang, Vipin Kumar, and Ju Sun, "Unlocking
195 inverse problems using deep learning: Breaking symmetries in phase retrieval," in *NeurIPS 2020 Workshop
196 on Deep Learning and Inverse Problems*, 2020.
- 197 [20] Raunak Manekar, Zhong Zhuang, Kshitij Tayal, Vipin Kumar, and Ju Sun, "Deep learning initialized phase
198 retrieval," in *NeurIPS 2020 Workshop on Deep Learning and Inverse Problems*, 2020.
- 199

- 200 [21] D. Russell Luke, Shoham Sabach, and Marc Teboulle, “Optimization on spheres: Models and proximal
201 algorithms with computational performance comparisons,” *SIAM Journal on Mathematics of Data Science*,
202 vol. 1, no. 3, pp. 408–445, jan 2019.
- 203 [22] S. Marchesini, “Invited article: A unified evaluation of iterative projection algorithms for phase retrieval,”
204 *Review of Scientific Instruments*, vol. 78, no. 1, pp. 011301, jan 2007.
- 205 [23] James R Fienup, “Phase retrieval algorithms: a comparison,” *Applied optics*, vol. 21, no. 15, pp. 2758–2769,
206 1982.
- 207 [24] D Russell Luke, “Relaxed averaged alternating reflections for diffraction imaging,” *Inverse problems*, vol.
208 21, no. 1, pp. 37, 2004.
- 209 [25] Veit Elser, “Phase retrieval by iterated projections,” *JOSA A*, vol. 20, no. 1, pp. 40–55, 2003.
- 210 [26] Jose A Rodriguez, Rui Xu, C-C Chen, Yunfei Zou, and Jianwei Miao, “Oversampling smoothness: an
211 effective algorithm for phase retrieval of noisy diffraction intensities,” *Journal of applied crystallography*,
212 vol. 46, no. 2, pp. 312–318, 2013.
- 213 [27] Stefano Marchesini, “Phase retrieval and saddle-point optimization,” *JOSA A*, vol. 24, no. 10, pp.
214 3289–3296, 2007.
- 215 [28] Zhong Zhuang, Gang Wang, Yash Travadi, and Ju Sun, “Phase retrieval via second-order nonsmooth
216 optimization,” in *ICML Workshop on Beyond First-Order Methods for Machine Learning*, 2020.
- 217 [29] S. Marchesini, H. He, H. N. Chapman, S. P. Hau-Riege, A. Noy, M. R. Howells, U. Weierstall, and J. C. H.
218 Spence, “X-ray image reconstruction from a diffraction pattern alone,” *Physical Review B*, vol. 68, no. 14,
219 pp. 140101, oct 2003.
- 220 [30] Ayan Sinha, Justin Lee, Shuai Li, and George Barbastathis, “Lensless computational imaging through deep
221 learning,” *Optica*, vol. 4, no. 9, pp. 1117–1125, 2017.
- 222 [31] Alexander Scheinker and Reemu Pokharel, “Adaptive 3d convolutional neural network-based reconstruction
223 method for 3d coherent diffraction imaging,” *Journal of Applied Physics*, vol. 128, no. 18, pp. 184901,
224 2020.
- 225 [32] Henry Chan, Youssef SG Nashed, Saugat Kandel, Stephan O Hruszkewycz, Subramanian KRS Sankara-
226 narayanan, Ross J Harder, and Mathew J Cherukara, “Rapid 3d nanoscale coherent imaging via physics-
227 aware deep learning,” *Applied Physics Reviews*, vol. 8, no. 2, pp. 021407, 2021.
- 228 [33] Ross Harder, “Deep neural networks in real-time coherent diffraction imaging,” *IUCrJ*, vol. 8, no. Pt 1, pp.
229 1, 2021.
- 230 [34] Longlong Wu, Shinjae Yoo, Ana F Suzana, Tadesse A Assefa, Jiecheng Diao, Ross J Harder, Wonsuk Cha,
231 and Ian K Robinson, “Three-dimensional coherent x-ray diffraction imaging via deep convolutional neural
232 networks,” *npj Computational Materials*, vol. 7, no. 1, pp. 1–8, 2021.
- 233 [35] Yudong Yao, Henry Chan, Subramanian Sankaranarayanan, Prasanna Balaprakash, Ross J Harder, and
234 Mathew J Cherukara, “Autophasenn: unsupervised physics-aware deep learning of 3d nanoscale bragg
235 coherent diffraction imaging,” *npj Computational Materials*, vol. 8, no. 1, pp. 1–8, 2022.
- 236 [36] Mathew J Cherukara, Youssef SG Nashed, and Ross J Harder, “Real-time coherent diffraction inversion
237 using deep generative networks,” *Scientific reports*, vol. 8, no. 1, pp. 1–8, 2018.
- 238 [37] Yuhe Zhang, Mike Andreas Noack, Patrik Vagovic, Kamel Fezzaa, Francisco Garcia-Moreno, Tobias
239 Ritschel, and Pablo Villanueva-Perez, “Phasegan: a deep-learning phase-retrieval approach for unpaired
240 datasets,” *Optics express*, vol. 29, no. 13, pp. 19593–19604, 2021.
- 241 [38] Christopher Metzler, Phillip Schniter, Ashok Veeraraghavan, et al., “prdeep: Robust phase retrieval with a
242 flexible deep network,” in *International Conference on Machine Learning*. PMLR, 2018, pp. 3501–3510.
- 243 [39] Çağatay Işıl, Figen S Oktem, and Aykut Koç, “Deep iterative reconstruction for phase retrieval,” *Applied
244 optics*, vol. 58, no. 20, pp. 5422–5431, 2019.
- 245 [40] Yaotian Wang, Xiaohang Sun, and Jason Fleischer, “When deep denoising meets iterative phase retrieval,”
246 in *International Conference on Machine Learning*. PMLR, 2020, pp. 10007–10017.
- 247 [41] Marcus C. Newton, Steven J. Leake, Ross Harder, and Ian K. Robinson, “Three-dimensional imaging of
248 strain in a single ZnO nanorod,” *Nature Materials*, vol. 9, no. 2, pp. 120–124, dec 2009.

- 249 [42] Dmitry Ulyanov, Andrea Vedaldi, and Victor Lempitsky, “Deep image prior,” *International Journal of*
250 *Computer Vision*, vol. 128, no. 7, pp. 1867–1888, 2020.
- 251 [43] Adnan Qayyum, Inaam Ilahi, Fahad Shamshad, Farid Boussaid, Mohammed Bennamoun, and Junaid
252 Qadir, “Untrained neural network priors for inverse imaging problems: A survey,” *IEEE Transactions on*
253 *Pattern Analysis and Machine Intelligence*, 2022.
- 254 [44] Taihui Li, Zhong Zhuang, Hengyue Liang, Le Peng, Hengkang Wang, and Ju Sun, “Self-validation: Early
255 stopping for single-instance deep generative priors,” *arXiv preprint arXiv:2110.12271*, 2021.
- 256 [45] Hengkang Wang, Taihui Li, Zhong Zhuang, Tiancong Chen, Hengyue Liang, and Ju Sun, “Early stopping
257 for deep image prior,” *arXiv preprint arXiv:2112.06074*, 2021.
- 258 [46] Zhong Zhuang, Taihui Li, Hengkang Wang, and Ju Sun, “Blind image deblurring with unknown kernel
259 size and substantial noise,” *arXiv preprint arXiv:2208.09483*, 2022.
- 260 [47] Reinhard Heckel and Mahdi Soltanolkotabi, “Denoising and regularization via exploiting the structural
261 bias of convolutional generators,” *arXiv preprint arXiv:1910.14634*, 2019.
- 262 [48] Reinhard Heckel and Mahdi Soltanolkotabi, “Compressive sensing with un-trained neural networks:
263 Gradient descent finds a smooth approximation,” in *International Conference on Machine Learning*.
264 PMLR, 2020, pp. 4149–4158.
- 265 [49] JN Clark, X Huang, R Harder, and IK Robinson, “High-resolution three-dimensional partially coherent
266 diffraction imaging,” *Nature communications*, vol. 3, no. 1, pp. 1–6, 2012.
- 267 [50] Felix Hofmann, Edmund Tarleton, Ross J Harder, Nicholas W Phillips, Pui-Wai Ma, Jesse N Clark, Ian K
268 Robinson, Brian Abbey, Wenjun Liu, and Christian E Beck, “3d lattice distortions and defect structures in
269 ion-implanted nano-crystals,” *Scientific reports*, vol. 7, no. 1, pp. 1–10, 2017.
- 270 [51] David Yang, Mark T Lapington, Guanze He, Kay Song, Minyi Zhang, Clara Barker, Ross J Harder, Wonsuk
271 Cha, Wenjun Liu, Nicholas W Phillips, et al., “Refinements for bragg coherent x-ray diffraction imaging:
272 Electron backscatter diffraction alignment and strain field computation,” *arXiv preprint arXiv:2203.17015*,
273 2022.
- 274 [52] Gijs Van Der Schot, Martin Svenda, Filipe RNC Maia, Max Hantke, Daniel P DePonte, M Marvin Seibert,
275 Andrew Aquila, Joachim Schulz, Richard Kirian, Mengning Liang, et al., “Imaging single cells in a beam
276 of live cyanobacteria with an x-ray laser,” *Nature communications*, vol. 6, no. 1, pp. 1–9, 2015.
- 277 [53] Yosef Gandelsman, Assaf Shocher, and Michal Irani, ““double-DIP”: Unsupervised image decomposi-
278 tion via coupled deep-image-priors,” in *2019 IEEE/CVF Conference on Computer Vision and Pattern*
279 *Recognition (CVPR)*. jun 2019, IEEE.
- 280 [54] Tobias Uelwer, Alexander Oberstraß, and Stefan Harmeling, “Phase retrieval using conditional generative
281 adversarial networks,” in *2020 25th International Conference on Pattern Recognition (ICPR)*. IEEE, 2021,
282 pp. 731–738.
- 283 [55] Tomoyoshi Shimobaba and Tomoyoshi Ito, *Computer Holography Acceleration Algorithms and Hardware*
284 *Implementations*, Taylor & Francis Group, 2019.

285 **A Failure of HIO when the support specification is loose**

286 The result is presented in Fig. 4.

287 **B Failure patterns of classical iterative methods on FFPR**

288 The result is presented in Fig. 5.

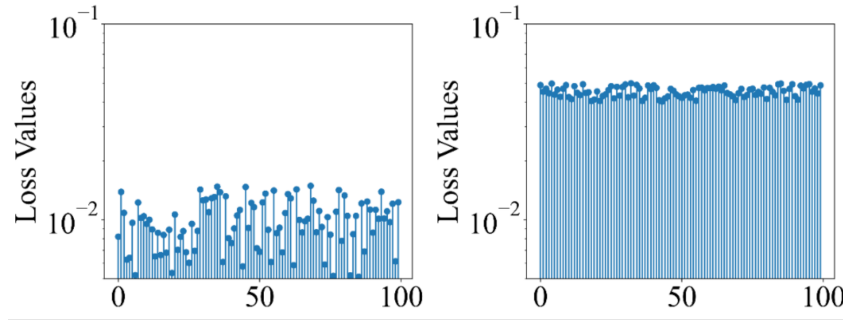


Figure 4: HIO to solve FFPR with vs without precise support. We plot the final least-squares losses over 100 random starts. X is the groundtruth in Fig. 1.

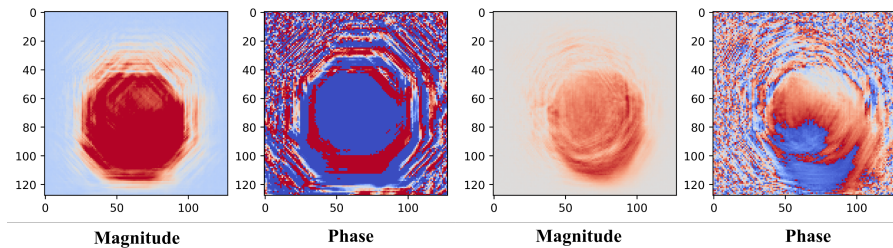


Figure 5: Two failure examples when solving FFPR using classical iterative methods without precise support specification and without shrinkwrap.

289 C Evaluation on 3D simulated Bragg CDI crystal data

290 We will not continue considering data-driven methods, due to their clear performance deficiency on
 291 2D data and the considerable cost to obtain sufficiently representative training sets for 3D. We only
 292 compare HES, which is the gold-standard used in Bragg CDI practice, with our double-DIP method.
 293 Since both methods can work with single instances and need no training data, here we quickly
 294 compare their performance qualitatively on a single 3D simulated crystal instance (the simulation
 295 process is similar to the 2D case), as shown in Fig. 6. It is obvious that even with Shrinkwrap
 296 iteratively refining support, HES still struggles to get the support right. By contrast, our double-DIP
 method obtains sharp support recovery and good phase estimation.

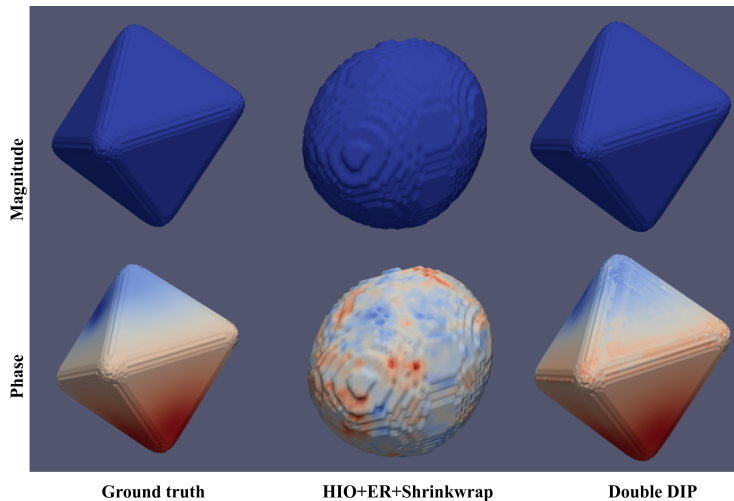


Figure 6: Visual comparison of reconstruction results by HIO+ER+Shrinkwrap and our method on a 3D simulated crystal instance

297 **D Fresnel and Fraunhofer approximations to the diffraction formula**

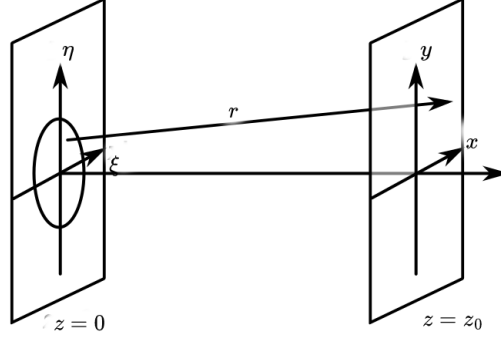


Figure 7: A schematic diffraction imaging system with parallel aperture and imaging planes (plot adapted from https://commons.wikimedia.org/wiki/File:Diffraction_geometry.svg under the Creative Commons Attribution-Share Alike 3.0 Unported license.)

298 In this section, we clarify the difference between the near-field and far-field models for phase retrieval,
 299 following [1, 55]. Consider the propagation of a monochromatic wave (with wavelength λ) from
 300 an aperture plane $z = 0$ to a parallel imaging plane $z = z_0$ with $z_0 \gg \lambda$; see Fig. 7. Let $U(x, y, z)$
 301 denote the wave field. The celebrated Rayleigh-Sommerfeld diffraction formula dictates that

$$U(x, y, z_0) = \frac{1}{2\pi} \iint U(\xi, \eta, 0) \left(\frac{1}{r(\xi, \eta)} - ik \right) \frac{z_0}{r^2(\xi, \eta)} e^{ikr(\xi, \eta)} d\xi d\eta, \quad (3)$$

302 where $r(\xi, \eta) \doteq \sqrt{z_0^2 + (x - \xi)^2 + (y - \eta)^2}$, $k \doteq \frac{2\pi}{\lambda}$ is the wavenumber, and the effective domain
 303 of the double integral is the aperture Ω . Moreover, write the domain of the image plane as $\Sigma \subset \mathbb{R}^2$.
 304 Eq. (3) has an equivalent form:

$$U(x, y, z_0) = \iint \widehat{U}(f_X, f_Y, 0) e^{ikz_0 \sqrt{1 - (\lambda f_X)^2 - (\lambda f_Y)^2}} e^{i2\pi(f_X x + f_Y y)} df_X df_Y, \quad (4)$$

305 where $\widehat{U}(f_X, f_Y, 0) = \iint U(x, y, 0) e^{-i2\pi(f_X x + f_Y y)} df_X df_Y$ is the 2D Fourier transform of the
 306 planar field $U(x, y, 0)$. The equivalence is due to the convolution theorem: write $r^\circ(x, y) \doteq$
 307 $\sqrt{z_0^2 + x^2 + y^2}$ and $h(x, y, z_0) \doteq \frac{1}{2\pi} \left(\frac{1}{r^\circ(x, y)} - ik \right) \frac{z_0}{[r^\circ(x, y)]^2} e^{ikr^\circ(x, y)}$. Then Eq. (3) can be writ-
 308 ten as $U(x, y, z_0) = U(x, y, 0) * h(x, y, z_0)$. The equivalence is clear once we recognize that
 309 $\widehat{r^\circ}(f_X, f_Y, z_0) \doteq \iint h(x, y, z_0) e^{-i2\pi(f_X x + f_Y y)} df_X df_Y = e^{ikz_0 \sqrt{1 - (\lambda f_X)^2 - (\lambda f_Y)^2}}$.

310 For Eq. (3), $\frac{1}{r(\xi, \eta)} - ik = \frac{1}{r(\xi, \eta)} - \frac{i2\pi}{\lambda} \approx \frac{2\pi}{i\lambda}$ as $r(\xi, \eta) \gg \lambda$ in practice. Hence we have the simplified
 311 form called the **Huygens-Fresnel principle**:

$$U(x, y, z_0) = \frac{z_0}{i\lambda} \iint U(\xi, \eta, 0) \frac{1}{r^2(\xi, \eta)} e^{ikr(\xi, \eta)} d\xi d\eta. \quad (5)$$

312 We can derive two approximations to Eq. (5), i.e., the Fresnel (i.e., near-field) and Fraunhofer (i.e.,
 313 far-field) approximations. Noting that $\sqrt{1 + \varepsilon} = 1 + \varepsilon/2 - \varepsilon^2/8 + O(\varepsilon^3)$ for $|\varepsilon| \ll 1$, we can
 314 approximate

$$r(\xi, \eta) \doteq \sqrt{z_0^2 + (x - \xi)^2 + (y - \eta)^2} = z_0 \sqrt{1 + \left(\frac{x - \xi}{z_0} \right)^2 + \left(\frac{y - \eta}{z_0} \right)^2} \quad (6)$$

315 by its low-order Taylor expansions, provided that $(x - \xi)^2 + (y - \eta)^2 \ll z_0^2$ for all $(\xi, \eta) \in \Omega$. First,
 316 we have $r^2(\xi, \eta) \approx z_0^2$ using only the 0-th order expansion. For the exponential term, since k is
 317 normally large, we use the 1-st order expansion:

$$\exp(ikr(\xi, \eta)) \approx \exp\left[ik\left(z_0 + \frac{(x - \xi)^2}{2z_0} + \frac{(y - \eta)^2}{2z_0}\right)\right] = e^{ikz_0} \exp\left[\frac{ik}{2z_0}((x - \xi)^2 + (y - \eta)^2)\right], \quad (7)$$

318 which is acceptable when

$$\frac{z_0 k}{8} \left(\left(\frac{x - \xi}{z_0} \right)^2 + \left(\frac{y - \eta}{z_0} \right)^2 \right)^2 \ll 1 \iff z_0^3 \gg \frac{k}{8} [(x - \xi)^2 + (y - \eta)^2]^2 \quad \forall (\xi, \eta) \in \Omega, (x, y) \in \Sigma. \quad (8)$$

319 So we arrive at the famous Fresnel approximation

$$\begin{aligned} U(x, y, z_0) &\approx \frac{e^{ikz_0}}{i\lambda z_0} \iint U(\xi, \eta, 0) \exp\left[\frac{ik}{2z_0}((x - \xi)^2 + (y - \eta)^2)\right] d\xi d\eta \\ &= \frac{e^{ikz_0}}{i\lambda z_0} e^{\frac{ik}{2z_0}(x^2 + y^2)} \iint [U(\xi, \eta, 0) e^{\frac{ik}{2z_0}(\xi^2 + \eta^2)}] e^{-\frac{ik}{z_0}(x\xi + y\eta)} d\xi d\eta. \end{aligned}$$

Fresnel approximation—forward

320 If moreover $\frac{ik}{2z_0}(\xi^2 + \eta^2) \ll 1 \iff z_0 \gg \frac{k}{2}(\xi^2 + \eta^2) \quad \forall (\xi, \eta) \in \Omega$, then $e^{\frac{ik}{2z_0}(\xi^2 + \eta^2)} \approx 1$ and
 321 hence we obtain:

$$U(x, y, z_0) \approx \frac{e^{ikz_0}}{i\lambda z_0} e^{\frac{ik}{2z_0}(x^2 + y^2)} \iint U(\xi, \eta, 0) e^{-\frac{ik}{z_0}(x\xi + y\eta)} d\xi d\eta.$$

Fraunhofer approximation—forward

322 By assuming $(\lambda f_X)^2 + (\lambda f_Y)^2 \ll 1$ and so $\sqrt{1 - (\lambda f_X)^2 - (\lambda f_Y)^2} \approx 1 - (\lambda f_X)^2/2 - (\lambda f_Y)^2/2$,
 323 we can approximate Eq. (4) as

$$U(x, y, z_0) \approx e^{ikz_0} \iint \widehat{U}(f_X, f_Y, 0) e^{-i\pi z_0 \lambda (f_X^2 + f_Y^2)} e^{i2\pi(f_X x + f_Y y)} df_X df_Y.$$

Fresnel approximation—backward

324 This is equivalent to the forward form of Fresnel approximation, due to

$$\mathcal{F}\left(\frac{1}{i\lambda z_0} e^{\frac{ik}{2z_0}(x^2 + y^2)}\right) = e^{-i\pi \lambda z_0 (f_X^2 + f_Y^2)}, \quad (9)$$

325 and the convolution theorem again.

326 So when we measure the field intensity on the image plane,

$$|U(x, y, z_0)|^2 \propto \left| \iint [U(\xi, \eta, 0) e^{\frac{ik}{2z_0}(\xi^2 + \eta^2)}] e^{-\frac{ik}{z_0}(x\xi + y\eta)} d\xi d\eta \right|^2 \quad (10)$$

$$\propto \left| \iint \widehat{U}(f_X, f_Y, 0) e^{-i\pi z_0 \lambda (f_X^2 + f_Y^2)} e^{i2\pi(f_X x + f_Y y)} df_X df_Y \right|^2 \quad (11)$$

327 according to the Fresnel (near-field) approximation, and

$$|U(x, y, z_0)|^2 \propto \left| \iint U(\xi, \eta, 0) e^{-\frac{ik}{z_0}(x\xi + y\eta)} d\xi d\eta \right|^2 \quad (12)$$

328 by the Fraunhofer (far-field) approximation. Detailed discussion of discretization and computation
 329 can be found in [1, Chapter 5].