Toward Practical Phase Retrieval with Deep Learning

Ju Sun Computer Science & Engineering, UMN

IPAM WS: Diffractive Imaging with Phase Retrieval, Oct 14, 2022



Thanks to

GLOVEX

https://glovex.umn.edu/



Taihui Li (CS&E)







Le Peng (CS&E)

Hengyue Liang (ECE)





Tiancong Chen (CS&E)

Thanks to







David Barmherzig CCM, Flatiron Ins.

Felix Hofmann DES, Oxford U. David Yang DES, Oxford U.





(Machine) Learning, (Numerical) Optimization, (Computer) Vision, healthcarE, +X





Our research themes

FOOLING THE AI

Deep neural networks (DNNs) are brilliant at image recognition — but they can be easily hacked.



Stop STOP + Stop Gaussian Noise Shot Noise Impulse Noise Defocus Blur Frosted Glass Blur





I: Trustworthy AI

III: AI for Healthcare





IV: AI for Science and Engineering

Which phase retrieval (PR)?

5 year ago...

UNIVERSITY OF MINNESOTA Driven to Discover⁵⁵



Home > Programs and Activities > Special V

- About
- Programs

Thematic Programs

Data Science

Hot Topics Workshops

Math-to-Industry Boot Camp

Public Lectures

Seminars

Special Workshops

Archived Programs



Mark Iwen	Michigan State University	
Rayan Saab	University of California, San Diego	
Aditya Viswanathan	Michigan State University	

Visiting

Which phase retrieval?



Miao et al. Beyond crystallography: Diffractive imaging using coherent x-ray light sources. Science, 2016 <u>https://www.science.org/doi/10.1126/science.aaa1394</u>

Are they created equal in difficulty levels?

 $oldsymbol{Y} = |\mathcal{A}(oldsymbol{X})|^2$ Consider $\min_{oldsymbol{X}} \|oldsymbol{Y} - |\mathcal{A}(oldsymbol{X})|^2\|_F^2$

	Gaussian PR	Fresnel PR	Fraunhofer PR
$\mathcal{A}(oldsymbol{X})$	$\{\langle oldsymbol{G}_i,oldsymbol{X} angle\}_{i=1}^m$	$\mathcal{F}(oldsymbol{X}\odot[e^{i\pi C(m^2+n^2)}]_{m,n}))$	$\mathcal{F}(oldsymbol{X})$
Symmetries	Global phase	Global phase	Shift, flipping, global phase

LS-solvable

un LS-solvable (proliferation of local mins) Focus of this talk:

plane-wave CDI (Fraunhofer PR) $Y = |\mathcal{F}(X)|^2$





Three symmetries: global phase conjugate flipping shift

When <u>deep learning (DL)</u> meets <u>visual inverse problems (VIPs)</u>

Visual inverse problems



Image denoising



Image super-resolution





3D reconstruction



MRI reconstruction



Coherent diffraction imaging (CDI)

Traditional methods

Inverse problem: given $\mathbf{y} = f(\mathbf{x})$, recover \mathbf{x}

$$\min_{\mathbf{x}} \underbrace{\ell(\mathbf{y}, f(\mathbf{x}))}_{\text{data fitting}} + \lambda \underbrace{R(\mathbf{x})}_{\text{regularizer}} \quad \mathsf{RegFit}$$

Limitations:

- Which ℓ ? (e.g., unknown/compound noise)
- Which R? (e.g., structures not amenable to math description)
- Speed

DL methods: the radical way

Inverse problem: given $\mathbf{y} = f(\mathbf{x})$, recover \mathbf{x} Learn the f^{-1} with a training set $\{(\mathbf{y}_i, \mathbf{x}_i)\}$



Limitations:

- Wasteful: not using f
- Representative data?
- Not always straightforward (see, e.g., Tayal et al. Inverse
 Problems, Deep Learning, and Symmetry Breaking. https://arxiv.org/abs/2003.09077)

Why symmetries hurt?



Symmetry breaking

Idea: process the training set to **break the symmetries** and hence minimize oscillations



Three symmetries: global phase, conjugate flipping, shift

Tayal et al. Unlocking Inverse Problems Using Deep Learning: Breaking Symmetries in Phase Retrieval. 2020 <u>https://sunju.org/pub/NIPS20-WS-DL4INV.pdf</u>

DL methods: the middle way

Inverse problem: given $\mathbf{y} = f(\mathbf{x})$, recover \mathbf{x}



Recipe: revamp numerical methods for RegFit with pretrained/trainable DNNs

DL methods: the middle way

Algorithm unrolling

$$\min_{\mathbf{x}} \underbrace{\ell(\mathbf{y}, f(\mathbf{x}))}_{ ext{data fitting}} + \lambda \underbrace{\operatorname{R}(\mathbf{x})}_{ ext{regularizer}}$$

If R proximal friendly

$$\mathbf{x}^{k+1} \,=\, \mathcal{P}_Rig(\mathbf{x}^k\,-\,\eta
abla^ op fig(\mathbf{x}^kig)\ell'ig(\mathbf{y},\,f(\mathbf{x}^k)ig)ig)$$

<u>Idea</u>: make \mathcal{P}_R trainable, using $\{(\mathbf{x}_i, \mathbf{y}_i)\}$



Fig credit: Deep Learning Techniques for Inverse Problems in Imaging https://arxiv.org/abs/2005.06001

DL methods: the middle way

Using $\{\mathbf{x}_i\}$ only

$$\min_{\mathbf{x}} \underbrace{\ell(\mathbf{y}, f(\mathbf{x}))}_{ ext{data fitting}} + \lambda \underbrace{\operatorname{R}(\mathbf{x})}_{ ext{regularizer}}$$

Plug-and-Play

$$\mathbf{x}^{k+1} \,=\, \mathcal{P}_Rig(\mathbf{x}^k\,-\,\eta
abla^ op fig(\mathbf{x}^kig)\ell'ig(\mathbf{y},\,f(\mathbf{x}^k)ig)ig)\,,$$

E.g. replace \mathcal{P}_R with pretrained denoiser

Deep generative models

DL methods: a survey

Deep Learning Techniques for Inverse Problems in Imaging

Gregory Ongie^{*}, Ajil Jalal[†], Christopher A. Metzler[‡] Richard G. Baraniuk[§], Alexandros G. Dimakis[¶], Rebecca Willett[∥]

April 2020

Abstract

Recent work in machine learning shows that deep neural networks can be used to solve a wide variety of inverse problems arising in computational imaging. We explore the central prevailing themes of this emerging area and present a taxonomy that can be used to categorize different problems and reconstruction methods. Our taxonomy is organized along two central axes: (1) whether or not a forward model is known and to what extent it is used in training and testing, and (2) whether or not the learning is supervised or unsupervised, i.e., whether or not the training relies on access to matched ground truth image and measurement pairs. We also discuss the tradeoffs associated with these different reconstruction approaches, caveats and common failure modes, plus open problems and avenues for future work. Focuses on **linear** inverse problems, i.e., f linear

https://arxiv.org/abs/2005.06001

Limitations of middle ways:

- Representative data?
- Algorithm-sensitive
 - Good initialization? (e.g., Manekar et al. **Deep Learning Initialized Phase Retrieval.**

https://sunju.org/pub/NIPS20-WS-DL4F PR.pdf)

DL methods: the **economic (radical)** way

Deep image prior (DIP) $\mathbf{x} pprox G_{ heta}\left(\mathbf{z}
ight)$ $G_{ heta}$ (and \mathbf{z}) trainable

 $egin{aligned} & \min_{\mathbf{x}} \, \underbrace{\ell(\mathbf{y},\,f(\mathbf{x}))}_{ ext{data fitting}} + \lambda \, \underbrace{\mathrm{R}(\mathbf{x})}_{ ext{regularizer}} & \mathbf{zero-training data!} \\ & & \parallel \ & \prod_{ ext{h}} \, \ell(\mathbf{y},\,f\circ G_{ heta}(\mathbf{z})) + \lambda R\circ G_{ heta}(\mathbf{z}) \end{aligned}$

Ulyanov et al. Deep image prior. IJCV'20. <u>https://arxiv.org/abs/1711.10925</u>

Contrasting: Deep generative models

Successes of DIP





Image denoising/inpainting/super-resol/deJEPG/...

https://dmitryulyanov.github.io/deep_image_prior

Blind image deblurring (blind deconvolution)

Ren et al. Neural Blind Deconvolution Using Deep Priors. CVPR'20. <u>https://arxiv.org/abs/1908.02197</u>



MRI reconstruction

Darestani and Heckel. Accelerated MRI with Un-trained Neural Networks. https://arxiv.org/abs/2007.02471 (ConvDecoder is a variant of DIP)



Phase retrieval

Tayal et al. Phase Retrieval using Single-Instance Deep Generative Prior. <u>https://arxiv.org/abs/2106.04812</u>



Surface reconstruction

Williams et al. Deep Geometric Prior for Surface Reconstruction. CVPR'19. <u>https://arxiv.org/abs/1811.10943</u>

Many others:

- PET reconstruction
- Audio denoising
- Time series

See recent survey

Oayyum et al.

Untrained neural network priors for inverse imaging problems: A survey. https://www.techrxiv.org/articles/preprint/Untrained_Neural_Network_Prio

rs_for_Inverse_Imaging_Problems_A_Survey/14208215

DIP's cousin(s)

Deep image prior (DIP)

 $\mathbf{x} pprox G_{ heta}\left(\mathbf{z}
ight) = G_{ heta}$ (and \mathbf{z}) trainable

Idea: (visual) objects as continuous functions

Neural implicit representation (NIR)

 $\mathbf{x} \approx \mathcal{D} \circ \overline{\mathbf{x}} \qquad \mathcal{D}: ext{discretization} \quad \overline{\mathbf{x}}: ext{ continuous function}$

Physics-informed neural networks (PINN)



Figure credit: https://www.nature.com/articles/s42254-021-00314-5

NIR for 3D rendering and view synthesis



https://www.matthewtancik.com/nerf

DIP for Practical PR





Alternating projection in action



Generalized alternating projection

- Hybrid input-output (HIO)
- Relaxed averaged alternating reflections (RAAR)
- Difference map
- Alternating direction of method of multiplier (ADMM)

See: Luke et al'19 https://doi.org/10.1137/18M1193025 Fannjiang & Strohmer'20 https://doi.org/10.1017/S096249292000069



Loose initial support? Shrinkwrap

Alternating projection in action



Beam stop

Limitations of SOTA methods on PR

Global issues

- Sensitivity to initial support estimation
- Sensitivity to multiple hyperparameters (e.g., Coherent Diffraction Imaging HIO+ER+Shrikwrap) (CDI)
- Low reconstruction quality (e.g., phases with singularities in BCDI)

Local issues

- Beamstop (i.e., missing data)
- Shot noise





Bragg Coherent Diffraction Imaging (BCDI)

Back to the LS formulation



$$\min_{\boldsymbol{X} \in \mathbb{C}^{n \times n}} \|\boldsymbol{Y} - |\mathcal{F}(\boldsymbol{X})|^2\|_F^2$$
$$\lim_{\boldsymbol{\theta}} \|\boldsymbol{Y} - |\mathcal{F} \circ G_{\boldsymbol{\theta}}(\boldsymbol{z})|^2\|_F^2$$

Single DIP doesn't work



Asymmetry between magnitude and complex phase

Double DIPs

$$\min_{oldsymbol{X}\in\mathbb{C}^{n imes n}} \|oldsymbol{Y}-|\mathcal{F}(oldsymbol{X})|^2\|_F^2$$

Reparameterizing X using two DIPs

$$\boldsymbol{X} = \boldsymbol{X}^{mag} e^{1j * \boldsymbol{X}^{phase}} = G_{\theta_1}^{mag} \left(z_1 \right) e^{1j * G_{\theta_2}^{phase} \left(z_2 \right)}$$

e.g., for BCDI on crystals, magnitude known to be uniform

OR
$$X = X^{real} + 1j * X^{imag} = G_{\theta_1}^{real}(z_1) + 1j * G_{\theta_2}^{imag}(z_2)$$

e.g., for CDI on certain bio-specimen, real part known to be nonnegative

X half of the size of Y in any dimension: no tight support needed

Zhuang et al. Practical Phase Retrieval Using Double Deep Image Priors. (Forthcoming)

Results on 2D simulated data

zero-training data!



Realistic 3D results (single-reflection)

slices from different views





Our



HIO+ER with Shrinkwrap

Yang et al. Application of single-instance deep generative priors for reconstruction of highly strained gold microcrystals in Bragg coherent X-ray diffraction. (Forthcoming)

Practical issues around DIP (and its cousin)





- 1) Early learning then overfitting (ELTO)
- 2) Slow in convergence
- 3) Which G_{θ} ?

Why early-learning-then-overfitting (ELTO)? $\min_{\theta} \ell(\mathbf{y}, f \circ G_{\theta}(\mathbf{z}))$

DIP learns signal **much faster than** learning noise



In practice, DIP heavily over-parameterized





Algorithm 1 DIP with ES–WMV

Input: random seed \boldsymbol{z} , randomly-initialized $G_{\boldsymbol{\theta}}$, window size W .
patience number P, empty queue Q , iteration counter $k = 0$
Output: reconstruction x^*
1: while not stopped do
2: update θ via Eq. (2) to obtain θ^{k+1} and x^{k+1}
3: push \boldsymbol{x}^{k+1} to \mathcal{Q} , pop queue front if $ \mathcal{Q} > W$
4: if $ \mathcal{Q} = W$ then
5: calculate VAR of elements in Q
6: update VAR _{min} and the corresponding x^*
7: if no decrease of VAR_{min} in <i>P</i> consecutive iterations
then
8: stop and return \boldsymbol{x}^k
9: end if Track running variance of estim
10: end if
11: $k = k + 1$
12: end while

Little over-head!

Table 5. Wall-clock time of DIP, SV-ES, ES-WMV and ES-EMV per epoch on *NVIDIA Tesla K40 GPU*: mean and (std).

	DIP	SV-ES	ES-WMV	ES-EMV
Time(secs)	0.448 (0.030)	13.027 (3.872)	0.301 (0.016)	0.003 (0.003)

- Li et al. Self-Validation: Early Stopping for Single-Instance Deep Generative Priors (BMVC'21) https://arxiv.org/abs/2110.12271
- Wang et al. Early Stopping for Deep Image Prior <u>https://arxiv.org/abs/2112.06074</u>

Acceleration—random projector (RP)

$$\min_{ heta} \, \ell(\mathbf{y}, \, f \circ G_{ heta}(\mathbf{z}))$$

Idea 1:

DIP: random z, trainable G RP: random G, trainable z

Idea 2: Reduce G, and put additional regularization $\min_{\theta} \ell(\mathbf{y}, f \circ G_{\theta}(\mathbf{z})) + \lambda R \circ G_{\theta}(\mathbf{z})$

Li et al. Random Projector: Toward Efficient Deep Image Prior. (forthcoming)

Blind deconvolution



Scanning tunneling microscopy (STM)



Cheung, Sky C., et al. "Dictionary learning in Fourier-transform scanning tunneling spectroscopy." *Nature communications* 11.1 (2020): 1-11. <u>https://www.nature.com/articles/s41467-020-14633-1</u>

Blind image deconvolution (BID)

y





 ∇y



x



 ∇x



k

Our recent work on BID

Tackle challenges about:

- Unknown kernel size
- Unknown noise type/level
- Both

$$\min_{\boldsymbol{k},\boldsymbol{x}} \underbrace{\ell(\boldsymbol{y},\boldsymbol{k}\ast\boldsymbol{x})}_{\text{data fitting}} + \underbrace{\lambda_{\boldsymbol{k}}R_{\boldsymbol{k}}(\boldsymbol{k})}_{\text{regularizing }\boldsymbol{k}} + \underbrace{\lambda_{\boldsymbol{x}}R_{\boldsymbol{x}}(\boldsymbol{x})}_{\text{regularizing }\boldsymbol{x}},$$

$$\min_{\boldsymbol{\theta}_{\boldsymbol{k}},\boldsymbol{\theta}_{\boldsymbol{x}}} \ell(\boldsymbol{y}, G_{\boldsymbol{\theta}_{\boldsymbol{k}}}(\boldsymbol{z}_{\boldsymbol{k}}) * G_{\boldsymbol{\theta}_{\boldsymbol{x}}}(\boldsymbol{z}_{\boldsymbol{x}})) + \lambda_{\boldsymbol{k}} R_{\boldsymbol{k}} \circ G_{\boldsymbol{\theta}_{\boldsymbol{k}}}(\boldsymbol{z}_{\boldsymbol{k}}) + \lambda_{\boldsymbol{x}} R_{\boldsymbol{x}} \circ G_{\boldsymbol{\theta}_{\boldsymbol{x}}}(\boldsymbol{z}_{\boldsymbol{x}}),$$

 Search...
 Help | Advance

 Electrical Engineering and Systems Science > Image and Video Processing
 Image Image

Blind image deblurring (BID) has been extensively studied in computer vision and adjacent fields. Modern methods for BID can be grouped into two categories: single-instance methods that deal with individual instances using statistical inference and numerical optimization, and data-driven methods that train deep-learning models to deblur future instances directly. Data-driven methods can be free from the difficulty in deriving accurate blur models, but are fundamentally limited by the diversity and quality of the training data -- collecting sufficiently expressive and realistic training data is a standing challenge. In this paper, we focus on single-instance methods that remain competitive and indispensable. However, most such methods do not prescribe how to deal with unknown kernel size and substantial noise, precluding practical deployment. Indeed, we show that several state-of-the-

Zhuang et al. Blind Image Deblurring with Unknown Kernel Size and Substantial Noise <u>https://arxiv.org/abs/2208.09483</u>

"ImageNet" for PR?



Original Shapes and Noisy Diffraction Patterns







/www.image-net.org/

Shapes: polygon, convex, nonconvex

Defects: varying number and density

~ 100K samples!

⁰ 150 250 Zhuang et al. **A realistic phase retrieval dataset**

for crystals. (Forthcoming)



min f(x) s.t. g(x) <= 0

Both f and g can be nonconvex, non-differentiable, **potentially involving deep neural networks**

Home

NCVX Package

ncvx.org

~

NCVX (NonConVeX) is a user-friendly and scalable python software package targeting general nonsmooth NCVX problems with nonsmooth constraints. NCVX is being developed by GLOVEX at the Department of Computer Science & Engineering, University of Minnesota, Twin Cities.

Our paper is available at https://arxiv.org/abs/2111.13984.

- Auto-differentiation
- GPU support
- Tensor variable support

Liang et al. NCVX: A General-Purpose Optimization Solver for Constrained Machine and Deep Learning.

https://arxiv.org/abs/2210.00973

Quick examples

$$\begin{split} \min_{\boldsymbol{w}, b, \zeta} \frac{1}{2} \|\boldsymbol{w}\|^2 + C \sum_{i=1}^n \zeta_i \\ \text{s.t.} \quad y_i \left(\boldsymbol{w}^{\intercal} \boldsymbol{x}_i + b \right) \geq 1 - \zeta_i, \ \zeta_i \geq 0 \ \forall i = 1, ..., n \end{split}$$

def comb fn(X struct): # obtain optimization variables w = X struct.w b = X struct. bzeta = X struct.zeta f = 0.5*w.T@w + C*torch.sum(zeta) ci = pygransoStruct() ci.cl = 1 - zeta - y*(x@w+b) ci.c2 = -zeta ce = None return [f,ci,ce] var in = {"w": [d,1], "b": [1,1], "zeta": [n,1]} soln = pygranso(var in,comb fn)

 $\max_{\boldsymbol{x}'} \quad \ell(\boldsymbol{y}, f_{\boldsymbol{\theta}}(\boldsymbol{x}'))$ s.t. $d(\boldsymbol{x}, \boldsymbol{x}') \leq \epsilon$ $\boldsymbol{x}' \in [0, 1]^n$

```
def comb fn(X struct):
    x prime = X struct.x prime
    f = loss func(y, f theta(x prime))
    ci = pygransoStruct()
    ci.cl = d(x, x prime) - epsilon
    ci.c2 = -x prime
   ci.c3 = x prime-1
    ce = None
    return [f,ci,ce]
var in = {"x prime": list(x.shape)}
soln = pygranso(var in,comb fn)
```

Papers

- Zhuang et al. Practical Phase Retrieval Using Double Deep Image Priors. (Forthcoming)
- Yang et al. Application of single-instance deep generative priors for reconstruction of highly strained gold microcrystals in Bragg coherent X-ray diffraction. (Forthcoming)
- Zhuang et al. A realistic phase retrieval dataset for crystals. (Forthcoming)

DIP at large

- Li et al. Self-Validation: Early Stopping for Single-Instance Deep Generative Priors (BMVC'21)
 https://arxiv.org/abs/2110.12271
- Wang et al. Early Stopping for Deep Image Prior https://arxiv.org/abs/2112.06074
- Zhuang et al. Blind Image Deblurring with Unknown Kernel Size and Substantial Noise. <u>https://arxiv.org/abs/2208.09483</u> (Submitted to IJCV)
- Li et al. Random Projector: Toward Efficient Deep Image Prior. (forthcoming)