Toward practical phase retrieval: to learn or not, and how to learn?

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CS&E, UMN

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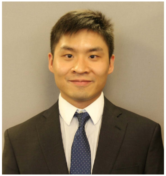


Gang Wang

UMN/BIT

Thanks to non-UMN folks

Stefano Marchesini

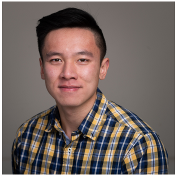
LBNL & Sigray, Inc.

David Barmherzig

CCM, Flatiron Ins.

Felix Hofmann

DES, Oxford U.



David Yang

DES, Oxford U.

Outline

Phase retrieval

Phase retrieval (PR): Given $|\mathcal{F}(\boldsymbol{x})|^2$, recover $\boldsymbol{x}$

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- $\mathcal{F}$: Fourier transform. Without $|\cdot|^2$, a matter of $\mathcal{F}^{-1}$!
- recover $\boldsymbol{x} \Longleftrightarrow$ recover $e^{i\angle\mathcal{F}(\boldsymbol{x})}$
- $\boldsymbol{x}$: 1D (vector), 2D (matrix), or 3D (tensor) signal

1D example: spectral factorization

In signal processing, control, and stochastic processes, etc: given an autocorrelation sequence $\boldsymbol{r} \in \mathbb{R}^{2n-1}$ and its Z transform $R(z)$

spectral factorization: given $R(z)$, find $X(z)$ so that $R(z) = \alpha X(z) X\left(z^{-1}\right)$ and $X(z)$ has all roots inside the unit circle.

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$\Longleftrightarrow$ find $\boldsymbol{x} \in \mathbb{R}^n$ given $\boldsymbol{r} = \boldsymbol{x} \star \boldsymbol{x}$

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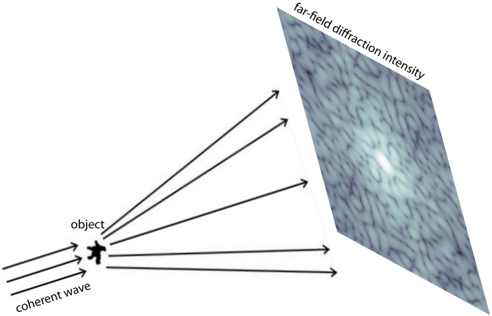
So: given $|\mathcal{F}(\boldsymbol{x})|^2$, recover $\boldsymbol{x}$— 1D PR!

[Sayed and Kailath, 2001, Barmherzig and Sun, 2018]

2D example: coherent diffraction imaging (CDI)



(Credit: [Shechtman et al., 2015])

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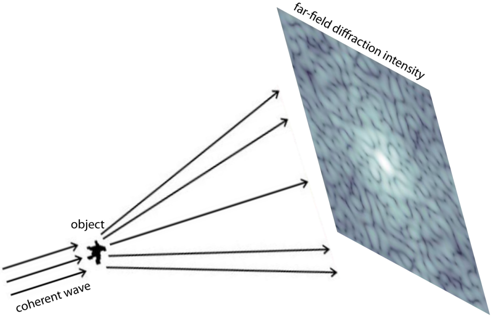

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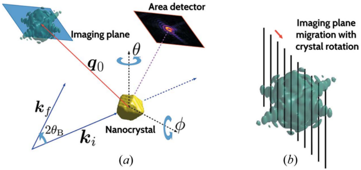
Fraunhofer (far-field) approximation:

$$|f(x,y)|^2 \approx \frac{1}{\lambda^2 z^2} \left| \widehat{I}\left(\frac{x}{\lambda z}, \frac{y}{\lambda z}\right) \right|^2,$$

where $I(x,y) = f(x,y,0)$ (complex-valued!).

3D example: Bragg coherent diffraction imaging (BCDI)



single-reflection BCDI

(Credit: [Maddali et al., 2020])

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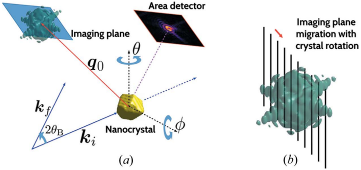

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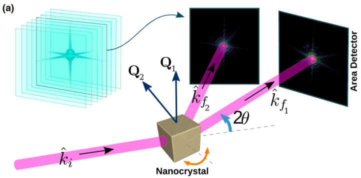

multi-reflection BCDI

(Credit: [Newton, 2020])

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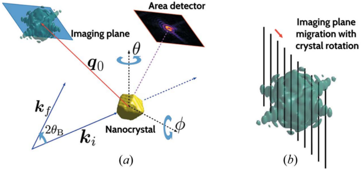

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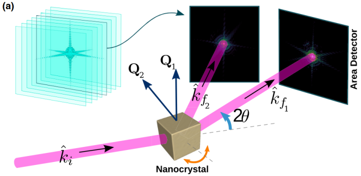

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(Credit: [Newton, 2020])

modern tools for x-ray crystallography, with application in chemistry, materials, medicine, etc

"Nobel-level problem"

 $\times 25$

Nobel Prizes involving X-ray crystallography [edit]

Year [hide]	Laureate	Prize	Rationale
1914	Max von Laue	Physics	"For his discovery of the diffraction of X-rays by crystals",[147] an important step in the development of X-ray spectroscopy.
1915	William Henry Bragg	Physics	"For their services in the analysis of crystal structure by means of X-rays"[148]
1915	William Lawrence Bragg	Physics	"For their services in the analysis of crystal structure by means of X-rays"[148]
1962	Max F. Perutz	Chemistry	"for their studies of the structures of globular proteins"[149]
1962	John C. Kendrew	Chemistry	"for their studies of the structures of globular proteins"[149]
1962	James Dewey Watson	Medicine	"For their discoveries concerning the molecular structure of nucleic acids and its significance for information transfer in living material"[150]
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1964	Dorothy Hodgkin	Chemistry	"For her determinations by X-ray techniques of the structures of important biochemical substances"[151]
1972	Stanford Moore	Chemistry	"For their contribution to the understanding of the connection between chemical structure and catalytic activity of the active centre of the ribonuclease molecule"[152]
1972	William H. Stein	Chemistry	"For their contribution to the understanding of the connection between chemical structure and catalytic activity of the active centre of the ribonuclease molecule"[152]
1976	William N. Lipscomb	Chemistry	"For his studies on the structure of boranes illuminating problems of chemical bonding"[153]
1985	Jerome Karle	Chemistry	"For their outstanding achievements in developing direct methods for the determination of crystal structures"[154]
1985	Herbert A. Hauptman	Chemistry	"For their outstanding achievements in developing direct methods for the determination of crystal structures"[154]
1988	Johann Deisenhofer	Chemistry	"For their determination of the three-dimensional structure of a photosynthetic reaction centre"[155]
1988	Hartmut Michel	Chemistry	"For their determination of the three-dimensional structure of a photosynthetic reaction centre"[155]
1988	Robert Huber	Chemistry	"For their determination of the three-dimensional structure of a photosynthetic reaction centre"[155]
1997	John E. Walker	Chemistry	"For their elucidation of the enzymatic mechanism underlying the synthesis of adenosine triphosphate (ATP)"[156]
2003	Roderick MacKinnon	Chemistry	"For discoveries concerning channels in cell membranes [...] for structural and mechanistic studies of ion channels"[157]
2003	Peter Agre	Chemistry	"For discoveries concerning channels in cell membranes [...] for the discovery of water channels"[157]
2006	Roger D. Kornberg	Chemistry	"For his studies of the molecular basis of eukaryotic transcription"[158]
2009	Ada E. Yonath	Chemistry	"For studies of the structure and function of the ribosome"[159]
2009	Thomas A. Steitz	Chemistry	"For studies of the structure and function of the ribosome"[159]
2009	Venkatraman Ramakrishnan	Chemistry	"For studies of the structure and function of the ribosome"[159]
2012	Brian Kobilka	Chemistry	"For studies of G-protein-coupled receptors"[160]

https://en.wikipedia.org/wiki/X-ray_crystallography#Nobel_Prizes_involving_X-ray_crystallography

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Possible at all?

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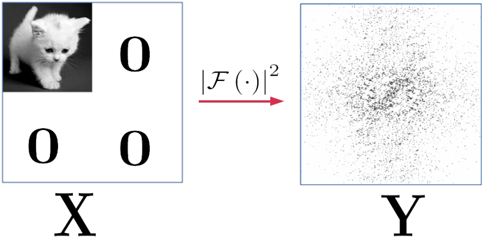

$\mathcal{F}$—oversampled Fourier transform

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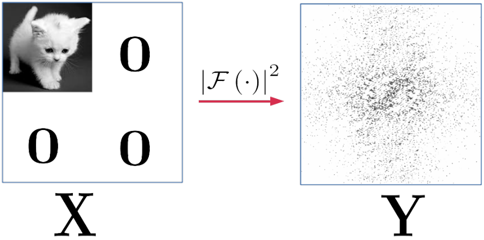

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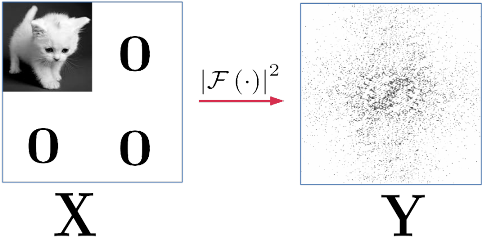

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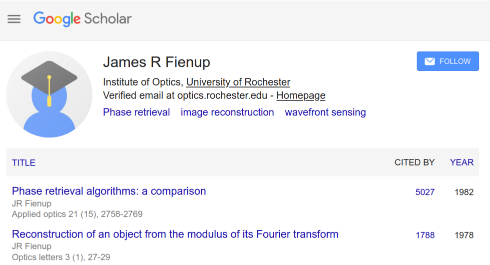
PR non-injective for 1D, but **generically** "injective" for 2D or higher [Hayes, 1982, Bendory et al., 2017]

- $\mathcal{M}$ constraint: $|\mathcal{F}(\boldsymbol{X})|^2 = \boldsymbol{Y}$
- $\mathcal{S}$ constraint: $\mathcal{A}(\boldsymbol{X}) = \mathbf{0}$

A brief history of PR algorithms

- Before 70's: error reduction method [Gerchberg and Saxton, 1972]
- Around 80's: hybrid input-output method [Fienup, 1982]



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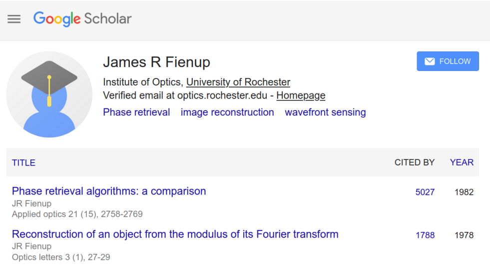
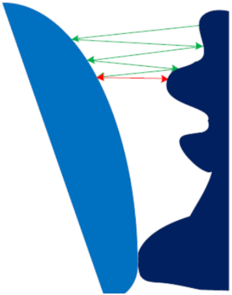


– Around 2000: connection to Douglas-Rachford method identified [Bauschke et al., 2002]
– Later variants: RAAR [Luke, 2004], difference map [Elser et al., 2007], see recent review [Luke et al., 2019]

PR algorithms

- Standard: alternating projection methods
- Popular: Fienup's hybrid input-output (HIO) and variants
- No guaranteed recovery (projection onto **nonconvex** sets)
- Often slow in practice, and sensitive to optimization parameters



Hybrid Input-Output (HIO) = Applying Douglas-Rachford splitting to $\delta_{\mathcal{M}} + \delta_{\mathcal{S}}$—ADMM! [Wen et al., 2012]

Insights from randomness?

(Fourier) phase retrieval:

For a complex signal $\boldsymbol{x} \in \mathbb{C}^n$, given $|\mathcal{F}\boldsymbol{x}|^2$, recover $\boldsymbol{x}$.

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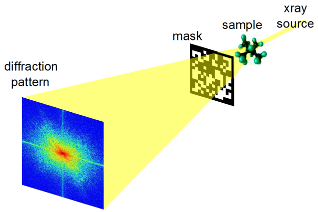

coded-diffraction

CDI [Candès et al., 2015]

Insights from the Gaussian case?

$\boldsymbol{y} = |\boldsymbol{a}_i^* \boldsymbol{x}|$ for $i = 1, \ldots, m$ where $\boldsymbol{a}_i$'s complex Gaussian vectors

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Example 1: a beautiful **init + local descent** result

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arXiv.org > cs > arXiv:1407.1065

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Phase Retrieval via Wirtinger Flow: Theory and Algorithms

Emmanuel Candes, Xiaodong Li, Mahdi Soltanolkotabi

(Submitted on 3 Jul 2014 (v1), last revised 24 Nov 2015 (this version, v3))

We study the problem of recovering the phase from magnitude measurements; specifically, we wish to reconstruct a complex-valued signal x of C^n about which we have phaseless samples of the form y_r = |< a_r,x >|^2, r = 1,2,...,m (knowledge of the phase of these samples would yield a linear system). This paper develops a non-convex formulation of the phase retrieval problem as well

Insights from the Gaussian case?

$\boldsymbol{y} = |\boldsymbol{a}_i^* \boldsymbol{x}|$ for $i = 1, \ldots, m$ where $\boldsymbol{a}_i$'s complex Gaussian vectors

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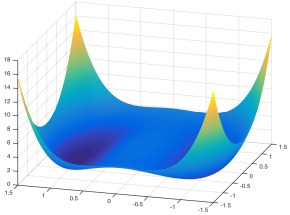
Example 2: my own results



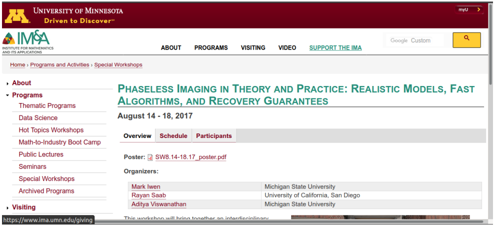
$$\min_{\boldsymbol{z} \in \mathbb{C}^n} f(\boldsymbol{z}) \doteq \frac{1}{2m} \sum_{k=1}^{m} (y_k^2 - |\boldsymbol{a}_k^* \boldsymbol{z}|^2)^2.$$

Theorem ([Sun et al., 2016])

When $\boldsymbol{a}_k$'s generic and m large, with high probability

all local minimizers are global, all saddles are nice.

I was happy until ...



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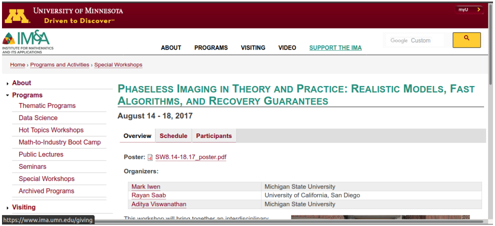

Take-home messages

James R Fienup

(U. Rochester)

I find it interesting people have tried to analyze Gaussian phase retrieval. —Fineup

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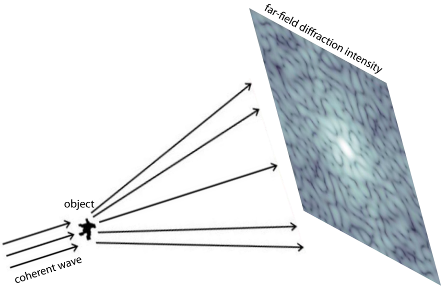
But we made little progress in solving Fourier PR

PR is about Fourier measurements



Fraunhofer (far-field) approximation:

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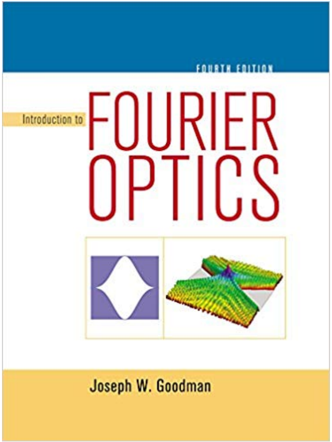
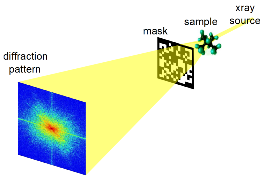


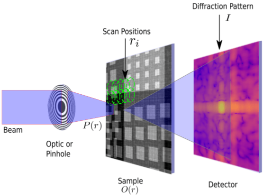
Variants of FPR

All variants are about Fourier measurements also

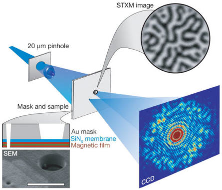
Coded diffraction



Ptychography



Fourier Holography



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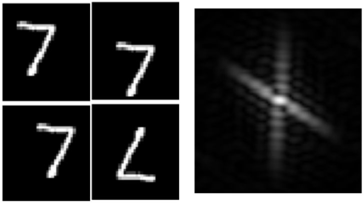

Symmetries in Fourier PR:

- translation
- 2D flipping
- global phase

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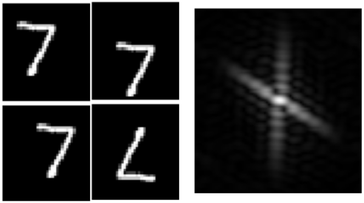

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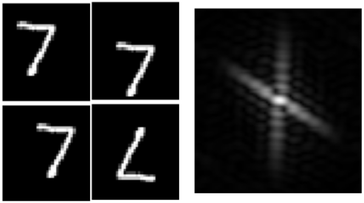

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> **Albert Einstein**: *Everything should be made as simple as possible, but no simpler.*

FPR remains difficult

- Most "natural" methods fail
  - Effective methods: **proximal methods** [Luke et al., 2019]
  - Exceptions: saddle point optimization [Marchesini, 2007, Pham et al., 2019], **2nd order ALM** [Zhuang et al., 2020]

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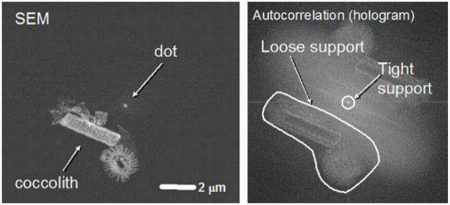

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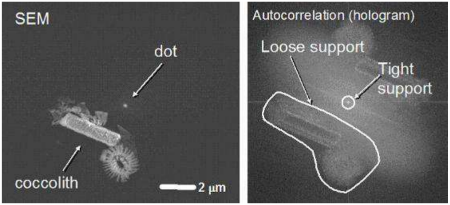

- Low-photon regime, beam stop, etc, e.g., [Chang et al., 2018]

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How people solve PR?

Deep learning for PR?

DL for inverse problems

Inverse problems: given $\boldsymbol{y} = f(\boldsymbol{x})$, estimate $\boldsymbol{x}$ (f may be unknown)

In FPR: $f = |\mathcal{F}(\cdot)|^2$

- Traditional

$$\min_{\boldsymbol{x}} \underbrace{\ell(\boldsymbol{y}, f(\boldsymbol{x}))}_{\text{data fidelity}} + \lambda \underbrace{\Omega(\boldsymbol{x})}_{\text{regularization}}$$

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  * End-to-end: set up $\{\boldsymbol{x}_i, \boldsymbol{y}_i\}$ to learn f^{-1} directly
  * Hybrid (model-based, physics-inspired, etc): replace ℓ, Ω, or algorithmic components using **learned functions**, e.g., plug-and-play ADMM, unrolling ISTA

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  * End-to-end: set up $\{\boldsymbol{x}_i, \boldsymbol{y}_i\}$ to learn f^{-1} directly
  * Hybrid (model-based, physics-inspired, etc): replace ℓ, Ω, or algorithmic components using **learned functions**, e.g., plug-and-play ADMM, unrolling ISTA
- "Modern" works **better** when "traditional" **already works**

DL for inverse problems

Inverse problems: given $\boldsymbol{y} = f(\boldsymbol{x})$, estimate $\boldsymbol{x}$ (f may be unknown)

In FPR: $f = |\mathcal{F}(\cdot)|^2$

- Traditional
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Recent surveys: [McCann et al., 2017, Lucas et al., 2018, Arridge et al., 2019, Ongie et al., 2020]

How?

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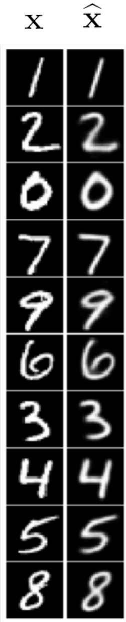
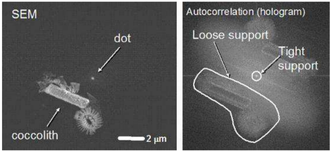
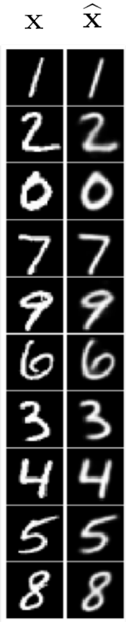
Focus here: **end-to-end approach**

How good are they?



but remember the practical hard cases and symmetries?





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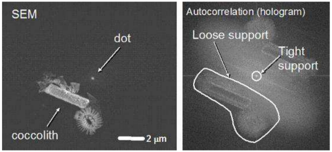

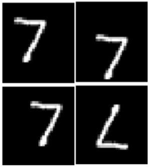

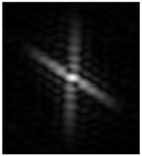

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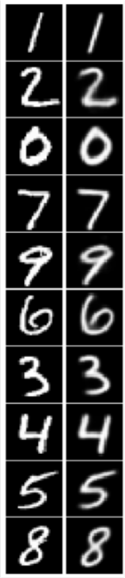
x $\hat{x}$



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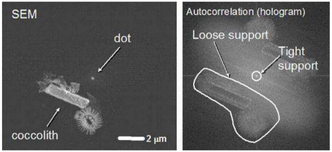
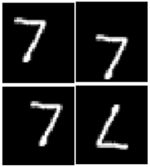
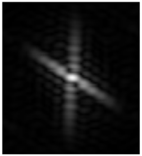
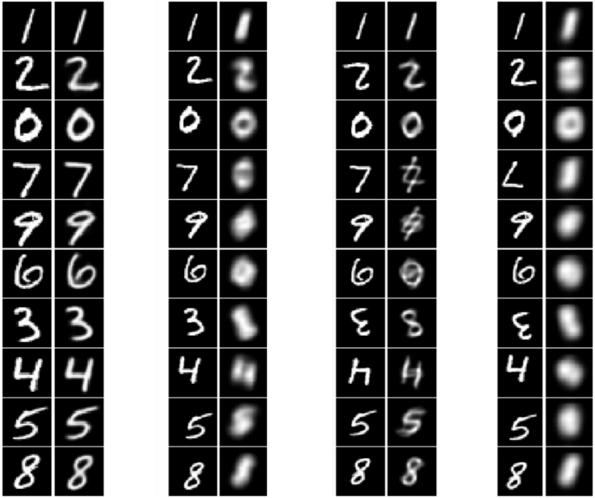






practical evaluation should account for the symmetries

Once we emulate the realistic symmetries



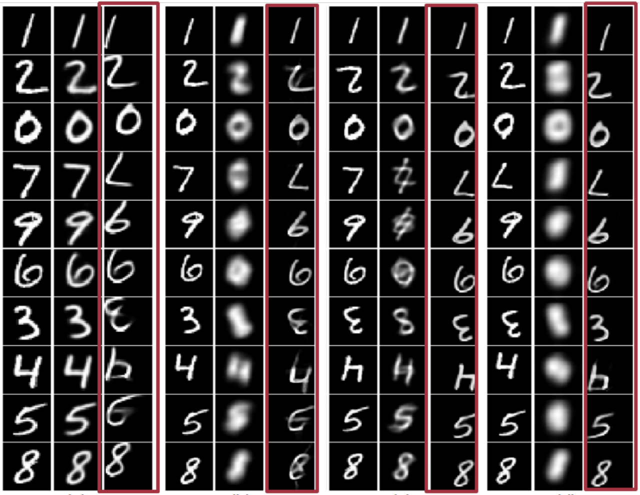
(a) No Symmetry

(b) Shift symmetry

(c) Flipping symmetry

(d) Shift and Flipping symmetries

Results using our methods



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Why (over)-optimistic results in practice?

Data! Data! Data!

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experimental data

naturally oriented and centered

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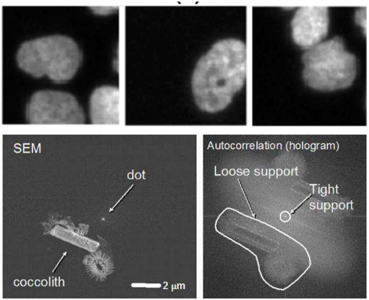

practical data

no natural orientation or centering

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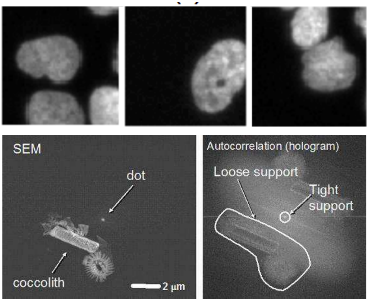

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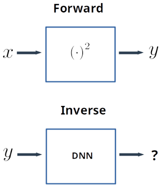
Dataset bias breaks problem symmetries

Why learning with symmetries is difficult?

Learning square roots!



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9	3
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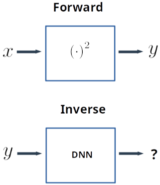

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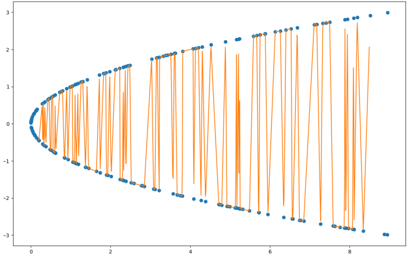

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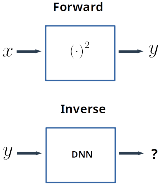

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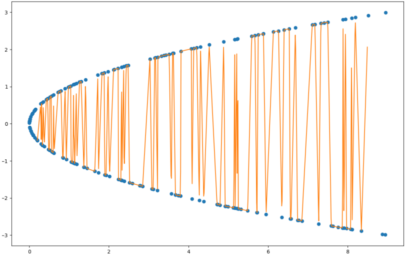

nearby inputs mapped to remote outputs **due to symmetries**

The difficulty is about one-to-many mapping

$\boldsymbol{y} = f(\boldsymbol{x})$ with f a many-to-one mapping

– symmetries in f

- **Fourier phase retrieval** [BBE17] The forward model is $\boldsymbol{Y} = |\mathcal{F}(\boldsymbol{X})|^2$, where $\boldsymbol{X} \in \mathbb{C}^{n\times n}$ and $\boldsymbol{Y} \in \mathbb{R}^{m\times m}$ are matrices and $\mathcal{F}$ is a 2D oversampled Fourier transform. The operation $|\cdot|$ takes complex magnitudes of the entries elementwise. It is known that translations and conjugate flippings applied on $\boldsymbol{X}$, and also global phase transfer of the form $e^{i\theta}\boldsymbol{X}$ all lead to the same $\boldsymbol{Y}$.
- **Blind deconvolution** [LG00, TB10] The forward model is $\boldsymbol{y} = \boldsymbol{a} \circledast \boldsymbol{x}$, where $\boldsymbol{a}$ is the convolution kernel, $\boldsymbol{x}$ is the signal (e.g., image) of interest, and $\circledast$ denotes the circular convolution. Both $\boldsymbol{a}$ and $\boldsymbol{x}$ are inputs. Here, $\boldsymbol{a} \circledast \boldsymbol{x} = (\lambda \boldsymbol{a}) \circledast (\boldsymbol{x}/\lambda)$ for any $\lambda \neq 0$, and circularly shifting $\boldsymbol{a}$ to the left and shifting $\boldsymbol{x}$ to the right by the same amount does not change $\boldsymbol{y}$.
- **Synchronization over compact groups** [PWBM18] For $g_1, \dots, g_n$ over a compact group $\mathcal{G}$, the observation is a set of pairwise relative measurements $y_{ij} = g_i g_j^{-1}$ for all (i,j) in an index set $\mathcal{E} \subset \{1, \dots, n\} \times \{1, \dots, n\}$. Obviously, any global shift of the form $g_k \mapsto g_k g$ for all $k \in \{1, \dots, n\}$, for any $g \in \mathcal{G}$, leads to the same set of measurements.

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Inverse f^{-1} is one-to-many mapping

Get rid of the difficulty?

- **active symmetry breaking**
- **passive symmetry breaking**

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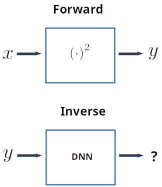
Details in

* **Deep Learning Initialized Phase Retrieval**. Manekar R, Tayal K, Kumar V, Sun J. NeurIPS 2020 Workshop on Deep Learning and Inverse Problems, 2020. https://sunju.org/pub/ICML20-WS-DL4FPR.pdf
* **Unlocking Inverse Problems Using Deep Learning: Breaking Symmetries in Phase Retrieval**. Tayal K, Lai C, Manekar R, Zhuang Z, Kumar V, Sun J. NeurIPS 2020 Workshop on Deep Learning and Inverse Problems, 2020. https://sunju.org/pub/ICML20-WS-DL4INV.pdf
* **Inverse Problems, Deep Learning, and Symmetry Breaking**. Tayal K, Lai C, Manekar R, Kumar V, Sun J. ICML workshop on ML Interpretability for Scientific Discovery, 2020. https://sunju.org/pub/ICML20-WS-DL4INV.pdf
* **Phase Retrieval via Second-Order Nonsmooth Optimization**. Zhuang Z, Wang G, Travadi Y, Sun J. ICML workshop on Beyond First Order Methods in Machine Learning, 2020.https://sunju.org/pub/ICML20-WS-ALM-FPR.pdf

An easy solution to the square root example



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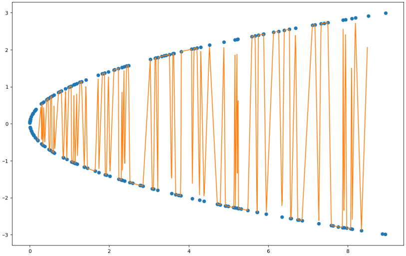

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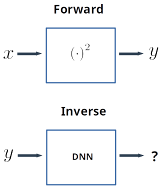

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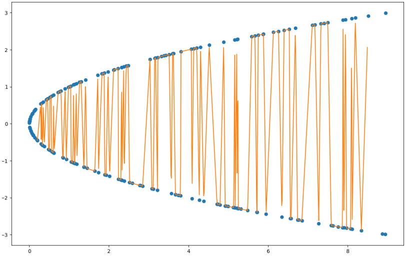

Modified Dataset

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64	8
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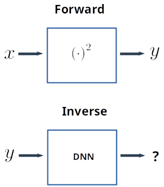

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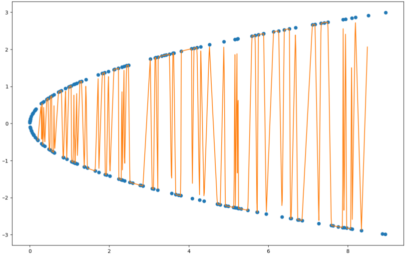

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idea: fix the sign symmetry

Active symmetry breaking

Real Gaussian PR: $\boldsymbol{y} = |\boldsymbol{A}\boldsymbol{x}|^2$ for illustration

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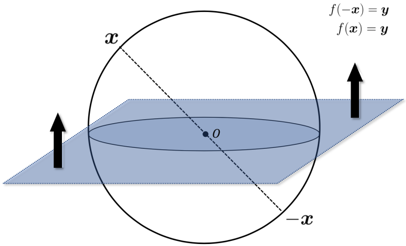

Active symmetry breaking

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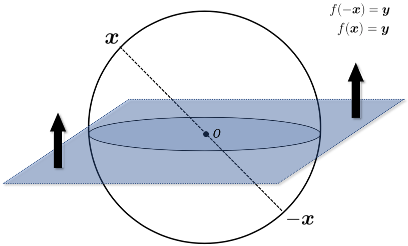


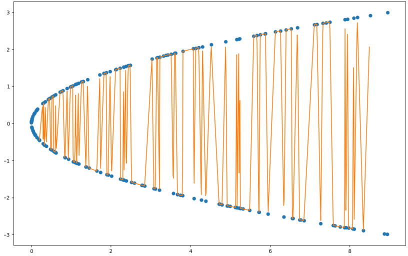
find a **smallest**, **representative**, and **connected** subset [Tayal et al., 2020]

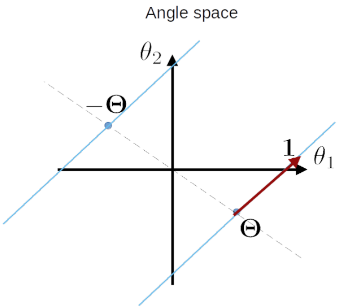
n	Sample	NN-A	K-NN	NN-B	WNN-A	K-NN	WNN-B	DNN-A	K-NN	DNN-B
5	2e4	10	17	283	**8**	18	283	10	19	284
	5e4	**6**	12	282	8	17	284	7	14	285
	1e5	**5**	10	284	**5**	12	283	13	18	284
	1e6	**4**	7	283	5	6	283	7	8	283
10	2e4	11	20	82	9	22	82	**8**	21	82
	5e4	9	16	82	**6**	18	82	9	20	82
	1e5	9	16	82	**6**	15	82	8	17	82
	1e6	7	13	82	**5**	10	82	9	11	82
15	2e4	12	17	38	**9**	16	38	**9**	16	38
	5e4	11	14	38	9	14	38	**8**	15	38
	1e5	10	13	38	8	13	38	**7**	13	38
	1e6	8	9	38	**7**	10	38	9	10	38

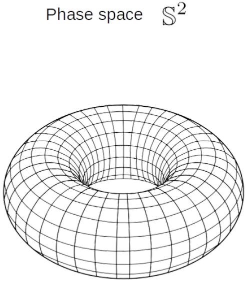
NN-A: **after** symmetry breaking

NN-B: **before** symmetry breaking—**denser sampling is worse**

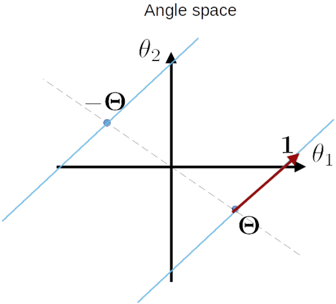
K-NN: K-nearest neighbor regression

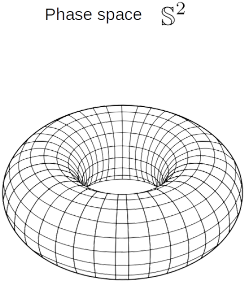



Angle space
θ_2
$-\Theta$
$\mathbf{1}$
θ_1
Θ


Phase space $\mathbb{S}^2$

Fourier PR

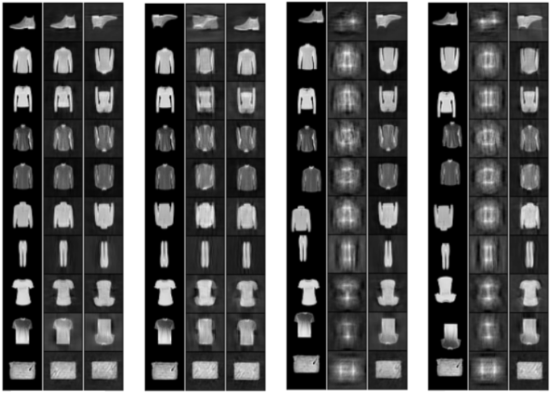




Pros: 1) math. principled 2) only symmetry info needed even if f unknown [Krippendorf and Syvaeri, 2020]

Cons: math. involved

Fourier PR



(a) No Symmetry (b) Flipping Symmetry (c) Shift Symmetry (d) Shift & Flipping Symmetry

Table 1: Test error using different symmetry schemes

	U-Net-B	U-Net-A (ours)
No Symmetry	0.103	0.103
Flipping Symmetry	0.168	0.162
Shift Symmetry	0.249	0.102
Shift & Flipping Symmetry	0.248	0.161

Table 2: MSE error

Method	MSE
ALM	0.299
U-Net-B	0.249
U-Net-A	0.160

Math-free alternative?

passive symmetry breaking

- If $\mathrm{DNN}_{\boldsymbol{W}}\left(\boldsymbol{y}_i\right) \approx \boldsymbol{x}_i$, then $\left|\mathcal{F} \circ \mathrm{DNN}_{\boldsymbol{W}}\left(\boldsymbol{y}_i\right)\right|^2 \approx \left|\mathcal{F} \boldsymbol{x}_i\right|^2 = \boldsymbol{y}_i$

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- Consider

$$\min_{\boldsymbol{W}} \sum_i \ell\left(\boldsymbol{y}_i, \left|\mathcal{F} \circ \mathrm{DNN}_{\boldsymbol{W}}\left(\boldsymbol{y}_i\right)\right|\right)$$

Math-free alternative?

passive symmetry breaking

- If $\mathrm{DNN}_{\boldsymbol{W}}\left(\boldsymbol{y}_i\right) \approx \boldsymbol{x}_i$, then $\left|\mathcal{F} \circ \mathrm{DNN}_{\boldsymbol{W}}\left(\boldsymbol{y}_i\right)\right|^2 \approx \left|\mathcal{F}\boldsymbol{x}_i\right|^2 = \boldsymbol{y}_i$
- Consider

$$\min_{\boldsymbol{W}} \sum_i \ell\left(\boldsymbol{y}_i, \left|\mathcal{F} \circ \mathrm{DNN}_{\boldsymbol{W}}\left(\boldsymbol{y}_i\right)\right|\right)$$

- Why it might work?
  * $\mathrm{DNN}_{\boldsymbol{W}}$ is simple when symmetries are broken
  * **implicit regularization** means simple $\mathrm{DNN}_{\boldsymbol{W}}$ is preferred

similar idea appears in [Metzler et al., 2020]

Practical variants

– Regularized version (when data sampling is sparse):

$$\min_{\boldsymbol{W}} \sum_i \ell\left(\boldsymbol{y}_i, \left|\mathcal{F} \circ \mathrm{DNN}_{\boldsymbol{W}}\left(\boldsymbol{y}_i\right)\right|\right) + \lambda \left\|\boldsymbol{J}_g\left(\boldsymbol{y}_i\right)\right\|_F^2$$

Practical variants

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- Refinement (with the support) using classic methods, e.g., 2nd order ALM [Zhuang et al., 2020]

Fourier PR

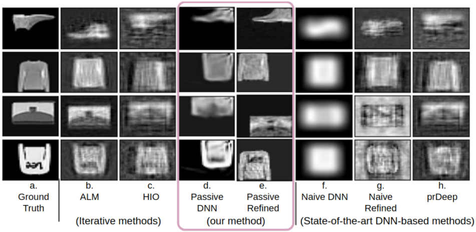

Table 1: MSE error

	MSE
ALM	0.312
HIO	0.441
Passive DNN	0.266
Passive Refined	0.187
Naive DNN	0.492
Naive Refined	0.397
prDeep	0.412

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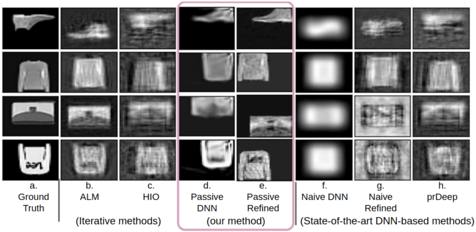

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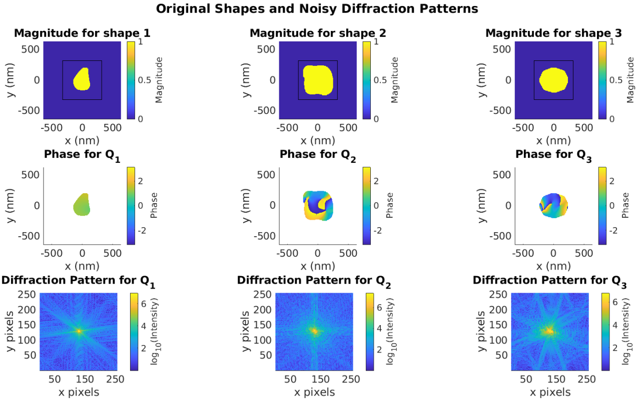
Pros: 1) lightweight 2) general

Cons: 1) f is needed 2) dense data needed

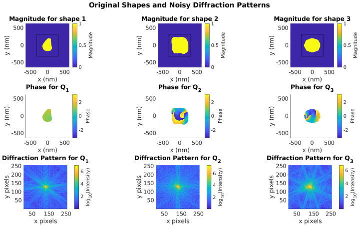
Current efforts

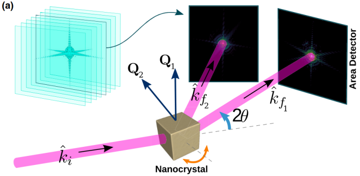
physically realistic datasets for Bragg CDI (270K data points)



in collaboration with Hofmann group at Oxford U.

physically realistic datasets for Bragg CDI (90K object instances)





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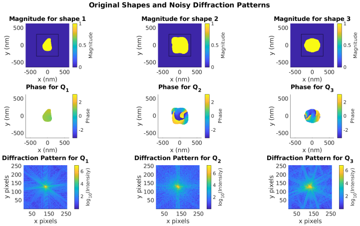
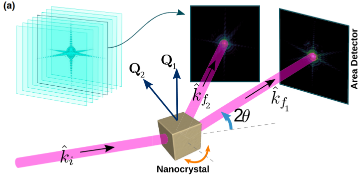




in collaboration with Hofmann group at Oxford U.

Bragg CDI is effectively a simultaneous FPR problem

Contribution

active and passive symmetry breaking for PR (and general inverse problems)

Contribution

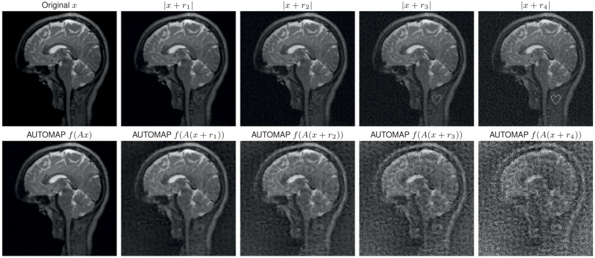
active and passive symmetry breaking for PR (and general inverse problems)

- End-to-end learning offers new opportunities for solving difficult PR instances
- Current successes are contaminated by dataset biases
- Symmetry breaking offers a way out

Thoughts

- Essential difficulty: use DL to approximate **one-to-many** mapping
  - When there is forward symmetry (this talk)
  - When the forward mapping under-determined (super-resolution, 3D structure from a single image)
  - or Both

- Essential difficulty: use DL to approximate **one-to-many** mapping
  - When there is forward symmetry (this talk)
  - When the forward mapping under-determined (super-resolution, 3D structure from a single image)
  - or Both
- Not only learning difficulty, but also **robustness** [Antun et al., 2020, Gottschling et al., 2020]



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