Ptychography: Theory & Algorithms

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Fannjiang-Strohmer, Acta Numerica (2020), 125-228.

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Coded-aperture phase retrieval



- Mask (wavefront) μ + propagation + intensity measurement: μ -coded diffraction pattern = $|\Phi(f \odot \mu)|^2$, Φ = Fourier transform.
- Ambiguities with one randomly coded diffraction pattern:

(harmless) constant phase translation conjugate inversion

$$f(\cdot) \longrightarrow e^{i\theta} f(\cdot)$$

$$f(\cdot) \longrightarrow f(\cdot + \mathbf{n})$$

$$f(\cdot) \longrightarrow \overline{f}(-\cdot)$$

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• Redundancy: 1+ randomly coded pattern.

Theorem (F. 2012)

Suppose f is a non-line object. Then the object is uniquely determined by two independent coded diffraction patterns up to a constant phase factor with probability one.

- Noise stability? $M \times N$ Gaussian measurement matrix: M = O(N)
 - $\rightarrow\,$ Candes-Strohmer-Voroninski 2013, Candes-Li 2014, Demanet-Hand 2014, Hand 2017
 - $\rightarrow\,$ PhaseMax: Goldstein-Studer 2018, Dhifallah-Thrampoulidis-Lu 2017

Numerics

- (Empirical) global convergence
 - \rightarrow Gradient-descent + special initialization methods: Alternating Projections (AP) or Wirtinger Flow (WF).
 - \rightarrow Initialization methods:
 - Spectral: Netrapalli-Jain-Sanghavi 2015, Chen-Candes 2017
 - Null-vector: Chen-F.-Liu 2017
 - Optimal spectral: Mondelli-Montanari 2019, Luo-Alghamdi-Lu 2019.



ightarrow Initialization methods are ineffective for blind phasing.

• ADMM/DRS: Globally and linearly convergent algorithm: Luke 2005, F.-Zhang 2020



• Convergence proof:

- \rightarrow Local convergence for the Fourier case with two diffraction patterns (Chen-F.-Liu 2017, Chen-F. 2018).
- \rightarrow Global convergence for suboptimal algorithms: Li-Pong 2016.
- → Global convergence for the Gaussian case with many diffraction patterns (Cand'es-Strohmer-Voroninski 2013, Candes-Li 2014, Candes-Li-Soltanolkotabi 2015).

Ptychography



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- Phase retrieval with windowed Fourier intensities.
- Measurement scheme:
 - \rightarrow Window function?
 - \rightarrow Scan pattern?
 - \rightarrow Overlap?

Mask/probe retrieval

Thibault et al. 08/09



- Relative residual reduces (from 32% to 18%) after mask recovery routine is turned on.
- Simultaneous recovery of the mask and the object?

Maiden-Johnson-Li 2017



• The mask is randomly initialized and the object is initialized as a constant.

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• Overlap ratio 70 - 80%.

- $\mathcal{T} \colon t \in \mathbb{Z}^2$ (pixel space) involved in ptychography.
- μ^0 the initial mask; μ^t the **t**-shifted mask
- $\mathcal{M}^0 = \mathbb{Z}^2_m$; $\mathcal{M}^{\mathbf{t}}$ the domain of $\mu^{\mathbf{t}}$.
- $\mathcal{M} := \cup_{t \in \mathcal{T}} \mathcal{M}^t$
- f^t : the object restricted to \mathcal{M}^t
- $\operatorname{Twin}(f^{\mathsf{t}})$: 180°-rotation of $\overline{f^{\mathsf{t}}}$ around the center of \mathcal{M}^{t}
- $f = \vee_{\mathbf{t}} f^{\mathbf{t}}$ with support $\subseteq \mathcal{M}$.

The original object is broken up into a set of overlapping object parts, each of which produces a coded diffraction pattern (coded by μ^{t}).

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Raster scan

Raster scan: $\mathbf{t}_{kl} = \tau(k, l), k, l \in \mathbb{Z}$ where τ is the step size. $\mathcal{M} = \mathbb{Z}_n^2, \ \mathcal{M}^0 = \mathbb{Z}_m^2, n > m$, with the periodic boundary condition.





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Measurement scheme

• $\mathcal{M}^t = \mathsf{nodes}$

• Two nodes are s-connected if $|\mathcal{M}^{\mathbf{t}} \cap \mathcal{M}^{\mathbf{t}'} \cap \operatorname{supp}(f)| \ge s \ge 2$.



Theorem (Chen-F. 2017)

Suppose that ptychographic graph is s-connected ($s \ge 2$). If the known mask comprises non-vanishing independent continuous random variables and every object part f^t is non-line, then the object is uniquely, up to a constant phase factor, by the ptychographic data.

Iwen-Viswanathan-Wang 2016: Uniqueness for standard raster scan with a standard Gabor window function shifted by one pixel at a time. 11/38

Graph representation







Raster scan with Fresnel mask can be ineffective



No uniqueness for a discrete set of ρ (except with one pixel shifts)! 300 13/38

Affine phase ambiguity

• Fundamental ambiguity with blind ptychography. Consider the probe and object estimates

$$\begin{split} \nu^0(\mathbf{n}) &= \mu^0(\mathbf{n}) \exp(-\mathrm{i} a - \mathrm{i} \mathbf{w} \cdot \mathbf{n}), \quad \mathbf{n} \in \mathcal{M}^0\\ g(\mathbf{n}) &= f(\mathbf{n}) \exp(\mathrm{i} b + \mathrm{i} \mathbf{w} \cdot \mathbf{n}), \quad \mathbf{n} \in \mathbb{Z}_n^2 \end{split}$$

for any $a, b \in \mathbb{R}$ and $\mathbf{w} \in \mathbb{R}^2$. Then

$$\nu^{\mathbf{t}}(\mathbf{n})g^{\mathbf{t}}(\mathbf{n}) = \mu^{\mathbf{t}}(\mathbf{n})f^{\mathbf{t}}(\mathbf{n})\exp(\mathrm{i}(b-a))\exp(\mathrm{i}\mathbf{w}\cdot\mathbf{t})$$

• $\exp(i\mathbf{w} \cdot \mathbf{t})$ depends on \mathbf{t} but not on $\mathbf{n} \Rightarrow g$ and ν^0 produce the same ptychographic data as f and μ^0 .

Phase drift

Necessary condition for blind ptychography:

$$(\star) \quad \nu^{\mathbf{t}} \odot g^{\mathbf{t}} = e^{\mathrm{i}\theta_{\mathbf{t}}} \mu^{\mathbf{t}} \odot f^{\mathbf{t}}, \quad \forall \mathbf{t} \in \mathcal{T},$$

for some θ_t (phase drift).

Theorem (F 2019)

Let $\mathcal{T} = \{t_k\}$ be a v-generated cyclic group of order q and M^k the t_k -shifted mask domain. Suppose that

$$u^k(\mathsf{n})g^k(\mathsf{n}) = e^{\mathrm{i} heta_k}\mu^k(\mathsf{n})f^k(\mathsf{n}), \quad \textit{for all } \mathsf{n} \in \mathcal{M}^k \textit{ and } \mathsf{t}_k \in \mathcal{T}.$$

lf

$$\mathcal{M}^k \cap \mathcal{M}^{k+1} \cap supp(f) \cap (supp(f) \oplus \mathbf{v}) \neq \emptyset, \quad \forall k$$

then $\{\theta_0, \theta_1, \ldots, \theta_{q-1}\}$ form an arithmetic progression.

Intermediate step

Theorem (F-Chen 2020)

Let the scheme be s-connected and each f^t is a non-line object. Suppose that some f^t has a tight support in \mathcal{M}^t and that $\mu^0 \neq 0$ has independently distributed random phases over at least the range of length π . Suppose that ν^0 with

$$(MPC) \quad \Re \Big[\overline{\nu^0}(\mathbf{n}) \mu^0(\mathbf{n}) \Big] > 0, \quad \forall \mathbf{n} \in \mathcal{M}^0,$$

and an arbitrary object $g = \bigcup_k g^k$ produce the same ptychographic data as f and μ^0 . Then the phase drift equation

$$(\star) \quad
u^{\mathbf{t}} \odot g^{\mathbf{t}} = e^{\mathrm{i} heta_{\mathbf{t}}} \mu^{\mathbf{t}} \odot f^{\mathbf{t}}, \quad orall \mathbf{t} \in \mathcal{T},$$

holds with probability at least $1 - c^s$, c < 1, where c depends on the mask phase distribution.

Object support constraint (OSC)

 f^{t} has a tight support in \mathcal{M}^{t} : Each and every side of \mathcal{M}^{t} intersects with $supp(f^{t})$.



OSC for a measurement scheme (the scan pattern): any translation of f would move some nonzero pixels across $\cup_t \partial \mathcal{M}^t$.

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OSC counter-example

Let
$$m = 2n/3$$
, $\mathbf{t} = (m/2, 0)$ $f^0 = [0, f_1^0]$ and $f^{\mathbf{t}} = [f_0^1, 0]$ with $f_1^0 = f_0^1$.
Likewise, $\mu^0 = [\mu_0^0, \mu_1^0], \mu^{\mathbf{t}} = [\mu_0^1, \mu_1^1]$.
Let $\nu^0 = \mu^0, \nu^{\mathbf{t}} = \mu^{\mathbf{t}}$ and $g^0 = [g_0^0, 0], g^{\mathbf{t}} = [0, g_1^1]$ where

$$\begin{array}{lll} g^0(\mathbf{n}) &=& \bar{f}^0(\mathbf{N}-\mathbf{n})\bar{\mu}^0(\mathbf{N}-\mathbf{n})/\mu^0(\mathbf{n}), & \forall \mathbf{n} \in \mathcal{M}^0\\ g^{\mathbf{t}}(\mathbf{n}) &=& \bar{f}^{\mathbf{t}}(\mathbf{N}+2\mathbf{t}-\mathbf{n})\bar{\mu}^{\mathbf{t}}(\mathbf{N}+2\mathbf{t}-\mathbf{n})/\mu^{\mathbf{t}}(\mathbf{n}), & \forall \mathbf{n} \in \mathcal{M}^{\mathbf{t}}. \end{array}$$

Hence $g^0 \odot \mu^0$ and $g^t \odot \mu^t$ produce the same diffraction patterns as $f^0 \odot \mu^0$ and $f^t \odot \mu^t$ but

$$\begin{array}{rcl} g^{0}\odot\mu^{0} & \neq & e^{\mathrm{i}\theta_{0}}f^{0}\odot\mu^{0} \\ g^{\mathrm{t}}\odot\mu^{\mathrm{t}} & \neq & e^{\mathrm{i}\theta_{\mathrm{t}}}f^{\mathrm{t}}\odot\mu^{\mathrm{t}} \end{array}$$

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even when the mask is completely known.

Block phase ambiguity

For
$$q = 3, \tau = m/2$$
, let

$$f = \begin{bmatrix} f_{00} & f_{10} & f_{20} \\ f_{01} & f_{11} & f_{21} \\ f_{02} & f_{12} & f_{22} \end{bmatrix}, \quad g = \begin{bmatrix} f_{00} & e^{i2\pi/3}f_{10} & e^{i4\pi/3}f_{20} \\ e^{i2\pi/3}f_{01} & e^{i4\pi/3}f_{11} & f_{21} \\ e^{i4\pi/3}f_{02} & f_{12} & e^{i2\pi/3}f_{22} \end{bmatrix}$$

be the object and its reconstruction, respectively, where $f_{ij}, g_{ij} \in \mathbb{C}^{n/3 \times n/3}$. Let

$$\mu^{kl} = \begin{bmatrix} \mu_{00}^{kl} & \mu_{10}^{kl} \\ \mu_{01}^{kl} & \mu_{11}^{kl} \end{bmatrix}, \quad \nu^{kl} = \begin{bmatrix} \mu_{00}^{kl} & e^{-i2\pi/3}\mu_{10}^{kl} \\ e^{-i2\pi/3}\mu_{01}^{kl} & e^{-i4\pi/3}\mu_{11}^{kl} \end{bmatrix}, \quad k, l = 0, 1, 2,$$

be the probe and its estimate, respectively, where $\mu_{ij}^{kl}, \nu_{ij}^{kl} \in \mathbb{C}^{n/3 \times n/3}$. $\implies \nu^{ij} \odot g^{ij} = e^{i(i+j)2\pi/3} \mu^{ij} \odot f^{ij}$.

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Periodic ambiguity (raster grid pathology)

 $(au=m/2)~{f t}_{kl}$ -shifted probes μ^{kl} and u^{kl} can be written as

$$\mu^{kl} = \begin{bmatrix} \mu_{00}^{kl} & \mu_{10}^{kl} \\ \mu_{01}^{kl} & \mu_{11}^{kl} \end{bmatrix}, \quad \nu^{kl} = \begin{bmatrix} \epsilon \odot \mu_{ij}^{kl} \end{bmatrix}$$

Let

$$\epsilon = [\alpha(\mathbf{n}) \exp(\mathrm{i}\phi(\mathbf{n}))], \quad \epsilon^{-1} = [\alpha^{-1}(\mathbf{n}) \exp(-\mathrm{i}\phi(\mathbf{n}))] \in \mathbb{C}^{\tau \times \tau}.$$

Consider the two objects

$$f = \begin{bmatrix} f_{00} & \dots & f_{q-1,0} \\ \vdots & \vdots & \vdots \\ f_{0,q-1} & \dots & f_{q-1,q-1} \end{bmatrix}, \quad g = \begin{bmatrix} \epsilon^{-1} \odot f_{ij} \end{bmatrix}$$

Two exit waves $\mu^{kl} \odot f^{kl}$ and $\nu^{kl} \odot g^{kl}$ are identical. But the estimates are far off.

Mixing schemes

- Rank-one perturbation $\mathbf{t}_{kl} = \tau(k, l) + (\delta_k^1, \delta_l^2)$.
- Full-rank perturbation $\mathbf{t}_{kl} = \tau(k, l) + (\delta_{kl}^1, \delta_{kl}^2).$





Global uniqueness

Theorem (F. 2019)

Suppose f does not vanish in \mathbb{Z}_n^2 . Let $a_j^i = 2\delta_{j+1}^i - \delta_j^i - \delta_{j+2}^i$ and let $\{\delta_{j_k}^i\}$ be the subset of perturbations satisfying $\operatorname{gcd}_{j_k}\{|a_{j_k}^i|\} = 1$, i = 1, 2, and

$$\begin{aligned} \tau &\geq \max_{i=1,2} \{ |a_{j_k}^i| + \delta_{j_k+1}^i - \delta_{j_k}^i \} \\ 2\tau &\leq m - \max_{i=1,2} \{ \delta_{j_k+2}^i - \delta_{j_k}^i \}, \quad (> 50\% \text{ overlap}) \\ m - \tau &\geq 1 + \max_{k'} \max_{i=1,2} \{ |a_{j_k}^i| + \delta_{k'+1}^i - \delta_{k'}^i \}. \end{aligned}$$

Then APA and SF are the only ambiguities, i.e. for some explicit r

$$g(\mathbf{n})/f(\mathbf{n}) = \alpha^{-1}(0) \exp(i\mathbf{n} \cdot \mathbf{r}),$$

$$\nu^{0}(\mathbf{n})/\mu^{0}(\mathbf{n}) = \alpha(0) \exp(i\phi(0) - i\mathbf{n} \cdot \mathbf{r}),$$

$$\theta_{kl} = \theta_{00} + \mathbf{t}_{kl} \cdot \mathbf{r}.$$

Theorem (F.-Chen 2020)

If ${\mathcal T}$ satisfies the mixing property, then

$$g(\mathbf{n})/f(\mathbf{n}) = \alpha^{-1}(0) \exp(i\mathbf{n} \cdot \mathbf{r}),$$

$$\nu^{0}(\mathbf{n})/\mu^{0}(\mathbf{n}) = \alpha(0) \exp(i\phi(0) - i\mathbf{n} \cdot \mathbf{r}),$$

$$\theta_{\mathbf{t}} = \theta_{0} + \mathbf{t} \cdot \mathbf{r}.$$

- Counterexamples exist for perturbed raster scans with < 50% overlap.
- Iwen-Preskitt-Saab-Viswanathan 2020: $\mathcal{T} = \mathbb{Z}_n^2 \Rightarrow$ noise stability.

Initialization with mask phase constraint

• Mask/probe initialization

 $\mu_1(\mathbf{n}) = \mu^0(\mathbf{n}) \exp{[i\phi(\mathbf{n})]},$

where $\phi(\mathbf{n})$ i.i.d. uniform on $(-\pi/2,\pi/2) \Longrightarrow$

$$\Re\Big[\overline{\mu_1}(\mathbf{n})\mu^0(\mathbf{n})\Big]>0,\quad \forall\mathbf{n}\in\mathcal{M}^0,$$



Relative error of the mask estimate

$$\sqrt{\frac{1}{\pi} \int_{-\pi/2}^{\pi/2} |e^{i\phi} - 1|^2 d\phi} = \sqrt{2(1 - \frac{2}{\pi})} \approx 0.8525$$

• Object initialization: $f_1 = \text{constant}$ or random phase object.

Noise-aware ADMM

- Let F(ν, x) = the totality of the Fourier (magnitude and phase) data for any mask ν and object x.
- Chang-Enfedaque-Marchesini 2019 consider the augmented Lagrangian

$$\mathcal{L}(\nu, x, z, \lambda) = \frac{1}{2} \|b - |z|\|^2 + \lambda^* (z - \mathcal{F}(\nu, x)) + \frac{\beta}{2} \|z - \mathcal{F}(\nu, x)\|^2$$

and the ADMM scheme

$$\mu_{k+1} = \arg \min \mathcal{L}(\nu, x_k, z_k, \lambda_k)$$

$$x_{k+1} = \arg \min \mathcal{L}(\mu_{k+1}, x, z_k, \lambda_k)$$

$$z_{k+1} = \arg \min \mathcal{L}(\mu_{k+1}, x_{k+1}, z, \lambda_k)$$

$$\lambda_{k+1} = \lambda_k + \beta(z_{k+1} - \mathcal{F}(\mu_{k+1}, x_{k+1})).$$

Fourier domain algorithms

• F.-Strohmer 2020 considers the augmented Lagrangian

$$\mathcal{L}(y, z, \lambda) = \frac{1}{2} ||z| - b||^2 + \lambda^*(z - y) + \frac{\rho}{2} ||z - y||^2 + \mathbb{I}_{\mathcal{F}}(y)$$

where $\mathbb{I}_{\mathcal{F}}$ is the indicator function of $\{y : y = \mathcal{F}(\nu, x) \text{ for some } \nu, x\}$.

$$\Rightarrow \begin{cases} (z_{k+1}, \mu_{k+1}) &= \arg \min_{z} \mathcal{L}(y_{k}, z, x_{k}, \nu, \lambda_{k}) \\ (y_{k+1}, x_{k+1}) &= \arg \min_{y} \mathcal{L}(y, z_{k+1}, x, \mu_{k+1}, \lambda_{k}) \\ \lambda_{k+1} &= \lambda_{k} + \rho(z_{k+1} - y_{k+1}) \end{cases}$$

$$\Rightarrow \begin{cases} z_{k+1} = \frac{1}{\rho+1} P_b(y_k - \lambda_k/\rho) + \frac{\rho}{\rho+1}(y_k - \lambda_k/\rho) \\ \mu_{k+1} = B_k^+ y_k \\ y_{k+1} = A_{k+1} A_{k+1}^+(z_{k+1} + \lambda_k/\rho) \\ x_{k+1} = A_{k+1}^+ y_{k+1} \quad (\text{needed for } B_{k+1}) \\ \lambda_{k+1}/\rho = \lambda_k/\rho + z_{k+1} - y_{k+1}. \end{cases}$$

where $A_{\nu}x := \mathcal{F}(\nu, x) = \text{concatenation of } \{ \Phi \operatorname{diag}(\nu^{\mathbf{t}}) \}$ and $B_{\mathbf{x}}\nu = \mathcal{F}(\nu, x) = \{ \Phi \operatorname{diag}(x^{\mathbf{t}}) \}$. Both have orthogonal columns.

In terms of the new variable $u_k = z_k + \lambda_{k-1}/\rho$, we have

$$u_{k+1} = \frac{1}{\rho+1} P_b(2A_kA_k^+u_k - u_k) + \frac{\rho}{\rho+1}(2A_kA_k^+u_k - u_k) + u_k - A_kA_k^+u_k$$

= $\frac{u_k}{\rho+1} + \frac{\rho-1}{\rho+1}A_kA_k^+u_k + \frac{1}{\rho+1}P_b(2A_kA_k^+u_k - u_k)$

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with $\mu_{k+1} = B_k^+ A_k A_k^+ u_k$, $x_{k+1} = A_{k+1}^+ u_{k+1}$.

Noise-agnostic ADMM

Consider

$$\mathcal{L}(z,\nu,x,\lambda) = \mathbb{I}_b(z) + \lambda^*(z - \mathcal{F}(\nu,x)) + \frac{1}{2} \|z - \mathcal{F}(\nu,x)\|^2$$

-

and the following ADMM scheme

$$z_{k+1} = \arg \min_{z} \mathcal{L}(z, \mu_k, x_k, \lambda_k) = P_b \left[\mathcal{F}(\mu_k, x_k) - \lambda_k \right]$$
$$(\mu_{k+1}, x_{k+1}) = \arg \min_{\nu} \mathcal{L}(z_{k+1}, \nu, x, \lambda_k)$$
$$\lambda_{k+1} = \lambda_k + z_{k+1} - \mathcal{F}(\mu_{k+1}, x_{k+1}).$$

If we simplify the bilinear optimization step by one-step alternating minimization

$$\mu_{k+1} = \arg \min_{\nu} \mathcal{L}(z_{k+1}, \nu, x_k, \lambda_k) = B_k^+(z_{k+1} + \lambda_k)$$

$$x_{k+1} = \arg \min_{g} \mathcal{L}(z_{k+1}, \mu_{k+1}, x, \lambda_k) = A_{k+1}^+(z_{k+1} + \lambda_k)$$

then we obtain the DM algorithm of Thibault et al. 2008/2009.

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eRAAR

Consider the augmented Lagrangian

$$\mathcal{L}(y, z, \nu, x, \lambda) = \mathbb{I}_{Y}(z) + \frac{1}{2} \|y - \mathcal{F}(\nu, x)\|^{2} + \lambda^{*}(z - y) + \frac{\gamma}{2} \|z - y\|^{2}$$

$$\Rightarrow \begin{cases} (y_{k+1}, x_{k+1}) &= \arg\min_{y} \mathcal{L}(y, z_{k}, x, \mu_{k}, \lambda_{k}) \\ (z_{k+1}, \mu_{k+1}) &= \arg\min_{z} \mathcal{L}(y_{k+1}, z, x_{k+1}, \nu, \lambda_{k}) \\ \lambda_{k+1} &= \lambda_{k} + \gamma(z_{k+1} - y_{k+1}). \end{cases}$$

In terms of the new variable $u_{k+1} := y_{k+1} - \lambda_k / \gamma$ and $R_b = 2P_b - I$

$$\Rightarrow \begin{cases} u_{k+1} = \beta u_k + (1 - 2\beta) P_b u_k + \beta P_k R_b u_k \\ \mu_{k+1} = B_{k+1}^+ (u_{k+1} + P_b u_k - u_k) \\ x_{k+1} = A_k^+ R_b u_k \end{cases}$$

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Test objects and error metric



 $\mathsf{RE}(k) = \min_{\alpha \in \mathbb{C}, \mathbf{k} \in \mathbb{R}^2} \frac{\|f(\mathbf{r}) - \alpha e^{-i\frac{2\pi}{n}\mathbf{k} \cdot \mathbf{r}} f_k(\mathbf{r})\|_2}{\|f\|_2}$ $\frac{\|f\|_2}{30 / 38}$

Scan patterns

- Rank-one perturbation $\mathbf{t}_{kl} = 30(k, l) + (\delta_k^1, \delta_l^2)$ where δ_k^1 and δ_l^2 are randomly selected integers in [-4, 4].
- Full-rank perturbation $\mathbf{t}_{kl} = 30(k, l) + (\delta_{kl}^1, \delta_{kl}^2)$ where δ_{kl}^1 and δ_{kl}^2 are randomly selected integers in [-4, 4].
- The adjacent probes overlap by roughly 50%.
- Boundary conditions:

Periodic BC Dark-field (enforced or not) Bright-field (enforced or not)



eGaussian-DRS vs eRAAR



Figure: eGaussian-DRS with $\rho = 1/3$ for CiB



Local convexity

• Let
$$L(Ax) := \|b - |Ax|\|$$
 and $B = \operatorname{diag}\left[\operatorname{sgn}(\overline{Ax})\right]A$.

(gradient)
$$2\Re[\zeta^*\nabla L(Ax)] = \Re(x^*\zeta) - b^{\top}\Re(B\zeta), \quad \forall \zeta \in \mathbb{C}^{n^2}$$

(stationarity) $B^*[|Ax| - b] = 0$

(Hessian) $\Re[\zeta^* \text{Hess}_x \zeta] = \|\zeta\|^2 - \Im(B\zeta)^T \operatorname{diag}\left[\frac{b}{|Ax|}\right] \Im(B\zeta).$

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Theorem (Chen-F. 2018)

Suppose f^t is not a line object for any t. For any connective scheme, the Hessian at x = f (nonvanishing almost surely) is positive semi-definite and the eigenvalue zero has multiplicity one.

Proof: the second largest singular value λ_2 of

$$\mathcal{B} = \begin{bmatrix} -\Re(B) & \Im(B) \end{bmatrix}$$

is strictly less than 1 with probability one.

Gaussian-DRS with known mask

• Fourier domain fixed points: $P_X = AA^+, R_X = 2P_X - I$ $P_X u + \rho P_X^{\perp} u = b \odot \operatorname{sgn}(R_X u).$

Theorem (F.-Zhang 2020)

Let u be a fixed point. (i) $\rho \ge 1$: If u is attracting, then $|P_X u| = b$ (i.e. regular solution). (ii) $\rho > 0$: If $|P_X u| = b$ then u is attracting. (iii) $\rho = 0$: local linear convergence near the true object

- DRS ($\rho \ge 1$): A fixed point is linearly attracting iff it is a true solution.
- DR ($\rho = 0$): continuously distributed unstable fixed points in the vicinity of the true solution \implies sub-linearly attracting.
- Convergence rate achieves the minimum

$$\frac{\lambda_2}{\sqrt{1+\rho_*}} \quad \text{at} \quad \rho_* = 2\lambda_2\sqrt{1-\lambda_2^2} \in [0,1].$$

Conclusion and Questions

Is Blind ptychography not realizable with the regular raster scan:

- ightarrow Mixing schemes: connective graph with overlap \geq 50%
- \rightarrow Mask prior: mask phase constraint.

Extension: 3D tomographic phase retrieval with uncertain orientations.



 Local convergence analysis for Gaussian-DRS with known mask. Global convergence: cf. Li-Pong 2016. Noise leads to infeasible optimization problem:

- Is Blind ptychography algorithms:
 - \rightarrow Little convergence analysis: cf. Hesse-Luke-Sabach-Tam 2015
 - \rightarrow Initialization method?

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References I

- Cand'es-Li 2014: "Solving quadratic equations via PhaseLift when there are about as many equations as unknowns", *Found. Comput. Math.* **14**, 10171026.
- Cand'es-Li-Soltanolkotabi 2015, "Phase retrieval from coded diffraction patterns", *Appl. Comput. Harmon. Anal.* **39**, 277299.
- Cand'es-Strohmer-Voroninski 2013: "PhaseLift: Exact and stable signal recovery from magnitude measurements via convex programming", *Commun. Pure Appl. Math.* **66**, 12411274.
- Chen-Cand'es 2017: "Solving random quadratic systems of equations is nearly as easy as solving linear systems", *Commun. Pure Appl. Math.* **70**, 822-883.
- Chen-Chi-Fan-Ma 2019: "Gradient descent with random initialization: Fast global convergence for nonconvex phase retrieval", *Math. Program.* **176**, 537.
- Chen-Fannjiang 2017: "Coded-aperture ptychography: Uniqueness and reconstruction," *Inverse Problems* **34**, 025003.
- Chen-Fannjiang 2018, "Phase retrieval with a single mask by Douglas-Rachford algorithms," *Appl. Comput. Harmon. Anal.* **44**, 665-699
- Chen-Fannjiang-Liu 2017: "Phase retrieval by linear algebra". SIAM Journal on Matrix Analysis and Applications **38** 854-868.
- Chen-Fannjiang-Liu 2018: "Phase retrieval with one or two diffraction patterns by alternating projections with the null initialization", *J. Fourier Anal. Appl.* 24, 24, 36/38

Ref. II

- Demanet-Hand 2014, "Stable optimizationless recovery from phaseless linear measurements," *J. Fourier Anal. Appl.* **20**, 199-221.
- Fannjiang 2012: "Absolute uniqueness of phase retrieval with random illumination," *Inverse Problems* **28** 075008.
- Fannjiang 2019: "Raster Grid Pathology and the Cure" *Multiscale Model. Simul.* **17**, 973-995.
- Fannjiang-Chen 2020: "Blind ptychography: Uniqueness & ambiguities," *Inverse Problems* **36**, 045005.
- Fannjiang-Strohmer 2020, "The numerics of phase retrieval," *Acta Numerica*, 125-228.
- Fannjiang-Zhang 2020: "Blind Ptychography by Douglas-Rachford Splitting," *SIAM J. Imaging Sci.* **13**, 609-650.
- Hand 2017, "PhaseLift is robust to a constant fraction of arbitrary errors", *Appl. Comput. Harmon. Anal.* **42**, 550-562.
- Hesse-Luke-Sabach-Tam 2015, "Proximal heterogeneous block implicit-explicit method and application to blind ptychographic diffraction imaging," SIAM J. Imaging Sci. 8, 426-457.
- Iwen-Preskitt-Saab-Viswanathan 2020: "Phase retrieval from local measurements: Improved robustness via eigenvector-based angular synchronization", *Appl.* 2000 *Comput. Harmon. Anal.* 48, 415-444. 37/38

Ref. III

- Iwen-Viswanathan-Wang 2016: "Fast phase retrieval from local correlation measurements", *SIAM J. Imaging Sci.*, **9**, 1655-1688.
- Li-Pong 2016, "Douglas-Rachford splitting for nonconvex optimization with application to nonconvex feasibility problems", *Math. Program.* A 159, 371-401
- Luke 2005, "Relaxed averaged alternating reflections for diffraction imaging," Inverse Problems 21, 37-50.
- Luo-Alghamdi-Lu 2019: "Optimal spectral initialization for signal recovery with applications to phase retrieval", *IEEE Trans. Signal Pro- cess.* 67, 2347-2356.
- Maiden-Johnson-Li 2017: "Further improvements to the ptychographical iterative engine", *Optica*, **4**, 736-745.
- Mondelli-Montanari 2019: "Fundamental limits of weak recovery with applications to phase retrieval", *Found. Comput. Math.* **19**, 703-773.
- Netrapalli-Jain-Sanghavi 2015: "Phase retrieval using alternating minimization," IEEE Transactions on Signal Processing 63 4814-4826.
- Thibault-Dierolf-Bunk-Menzel-Pfeiffer 2009: "Probe retrieval in ptychographic coherent diffractive imaging", *Ultramicroscopy* **109**, 338-343.
- Thibault-Dierolf-Menzel-Bunk-David-Pfeiffer 2008: "High-resolution scanning x-ray diffraction microscopy", Science 321, 379-382.