Blind Ptychography: Theory & Algorithms

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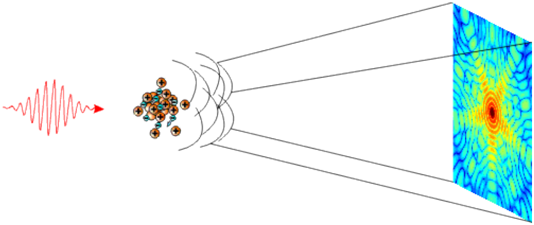
Outline

- Introduction and motivation: Phase retrieval vs. ptychography.
- Mathematical set-up
- Inherent ambiguities
- Local uniqueness of the exit waves
- Raster grid pathology
- Global uniqueness for mixing schemes.
- Reconstruction
- Conclusion

Phase retrieval

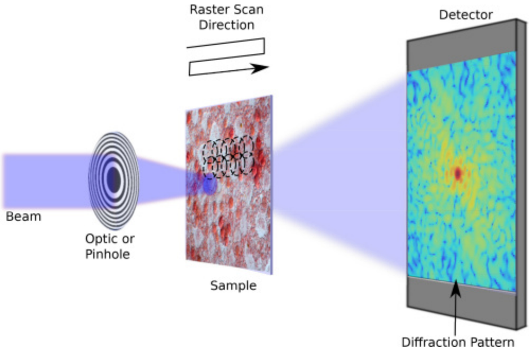


- Mask/probe μ + propagation $\mathcal{F}$ + intensity measurement:

$$\text{data} = \text{diffraction pattern} = |\mathcal{F}(f \otimes \mu)|^2, \quad \mathcal{F} = \text{Fourier transform.}$$

Ptychography: extended objects

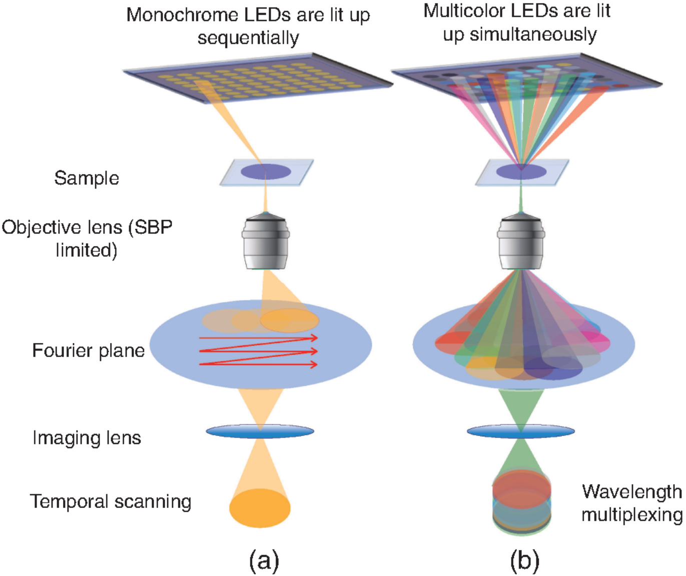
Hoppe (1969): electron microscopy.



- Inverse problem with windowed Fourier intensities.

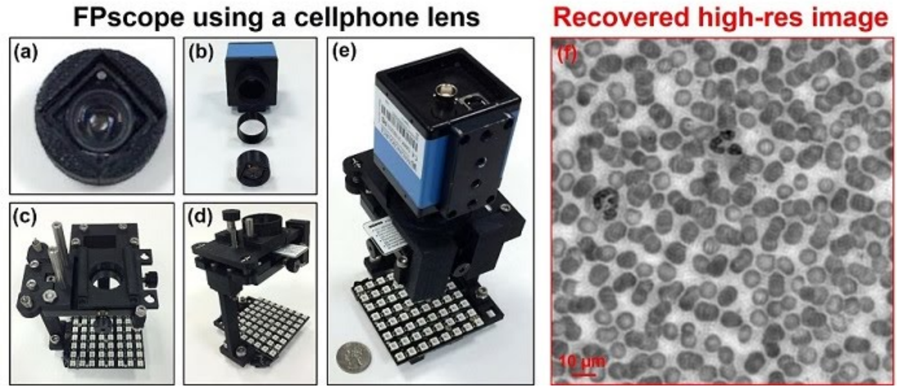
Fourier ptychography

Zheng *et al.* (2013): Convolution in the Fourier domain.



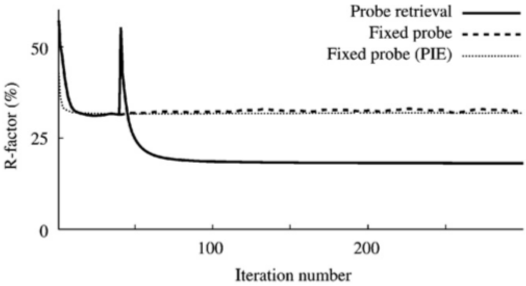
Fourier ptychography

Zheng *et al.* (2014)



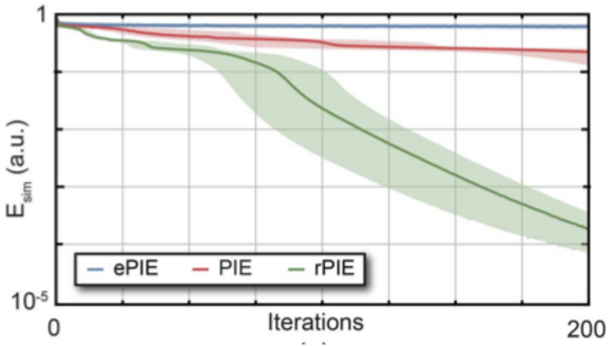
Mask/probe retrieval

Thibault *et al.* (08/09) - Lensless coherent diffractive imaging



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

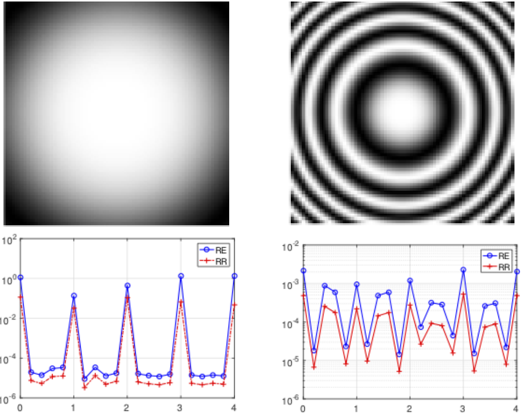
Maiden et al. 2017



- A randomly masked aperture of approximately the same size as the true probe was used as an initial probe estimate and free-space was used as the initial object estimate.
- Overlap ratio $70 - 80\%$.

Twin image ambiguity: Chen & F (2017)

Fresnel mask $\mu^0(\mathbf{k}) := \exp\left\{ \mathrm{i}\pi\rho|\mathbf{k}|^2/m \right\}$



(a) $q = 2$ (b) $q = 4$

No uniqueness for certain ρ even if the mask is known!

Notation & set-up

- $\mathcal{T}$: all the shifts $\mathbf{t} \in \mathbb{Z}^2$ involved in the measurement.
- μ^0 the initial mask; $\mu^{\mathbf{t}}$ the $\mathbf{t}$-shifted mask
- $\mathcal{M}^0 = \mathbb{Z}_m^2$; $\mathcal{M}^{\mathbf{t}}$ the domain of $\mu^{\mathbf{t}}$.
- $\mathcal{M} := \cup_{\mathbf{t}\in\mathcal{T}} \mathcal{M}^{\mathbf{t}}$
- $f^{\mathbf{t}}$: the object restricted to $\mathcal{M}^{\mathbf{t}}$
- $\mathrm{Twin}(f^{\mathbf{t}})$: 180°-rotation of $\overline{f^{\mathbf{t}}}$ around the center of $\mathcal{M}^{\mathbf{t}}$
- $f = \vee_{\mathbf{t}} f^{\mathbf{t}} \subseteq \mathcal{M}$ and refer to each $f^{\mathbf{t}}$ as a part of f.

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

Linear phase ambiguity

Consider the probe and object estimates

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

for any $a, b \in \mathbb{R}$ and $\mathbf{w} \in \mathbb{R}^2$. For any $\mathbf{t}$, we have the following calculation

$$\begin{aligned} \nu^{\mathbf{t}}(\mathbf{n}) &= \nu^0(\mathbf{n}-\mathbf{t}) \\ &= \mu^0(\mathbf{n}-\mathbf{t}) \exp(-\mathrm{i}\mathbf{w}\cdot(\mathbf{n}-\mathbf{t})) \exp(-\mathrm{i}a) \\ &= \mu^{\mathbf{t}}(\mathbf{n}) \exp(-\mathrm{i}\mathbf{w}\cdot(\mathbf{n}-\mathbf{t})) \exp(-\mathrm{i}a) \end{aligned}$$

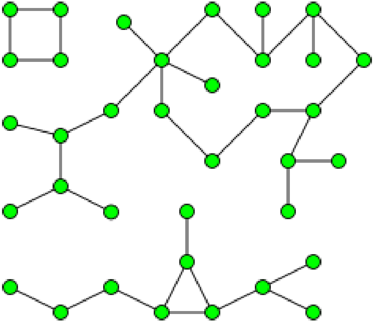
and hence for all $\mathbf{n} \in \mathcal{M}^{\mathbf{t}}, \mathbf{t} \in \mathcal{T}$

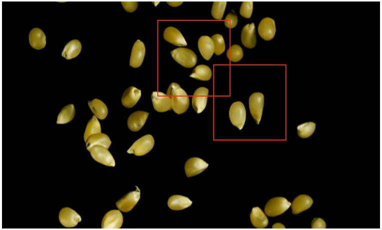
$$\nu^{\mathbf{t}}(\mathbf{n}) g^{\mathbf{t}}(\mathbf{n}) = \mu^{\mathbf{t}}(\mathbf{n}) f^{\mathbf{t}}(\mathbf{n}) \exp(\mathrm{i}(b-a)) \exp(\mathrm{i}\mathbf{w}\cdot\mathbf{t})$$

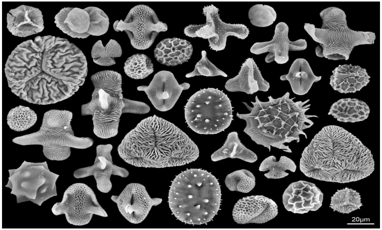
implying g and ν^0 produce the same ptychographic data as f and μ^0 since for each $\mathbf{t}$, $\nu^{\mathbf{t}} \odot g^{\mathbf{t}}$ is a constant phase factor times $\mu^{\mathbf{t}} \odot f^{\mathbf{t}}$.

Measurement scheme

- $\mathcal{M}^{\mathbf{t}} =$ nodes
- Two nodes are s-connected if $|\mathcal{M}^{\mathbf{t}} \cap \mathcal{M}^{\mathbf{t}'} \cap \text{supp}(f)| \geq s$.





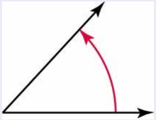


Block phase

Theorem (F & Chen 2018)

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

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



and an arbitrary object $g = \cup_k g^k$ produce the same ptychographic data as f and μ^0. Then with probability at least $1 - c^s$, $c < 1$,

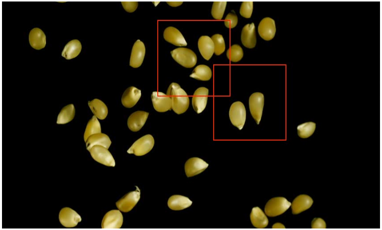
$$\nu^{\mathbf{t}} \odot g^{\mathbf{t}} = e^{i\theta_{\mathbf{t}}} \mu^{\mathbf{t}} \odot f^{\mathbf{t}}, \quad \forall \mathbf{t} \in \mathcal{T},$$

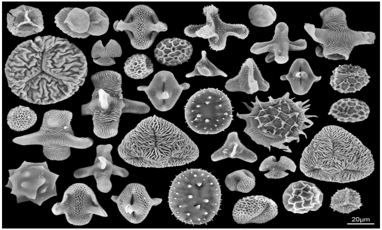
where c depends on the mask phase distribution.

$\theta_{\mathbf{t}}$ = block phases depending on $\mathbf{t}$ but not $\mathbf{n}$.

Object support constraint (OSC)

$f^{\mathbf{t}}$ has a tight support in $\mathcal{M}^{\mathbf{t}}$: $\mathcal{M}^{\mathbf{t}}$ is the smallest rectangle containing $f^{\mathbf{t}}$.





OSC is a relaxation of the tight support condition.

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

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

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

$$\begin{aligned} g^0 \odot \mu^0 &\neq e^{i\theta_0} f^0 \odot \mu^0 \\ g^{\mathbf{t}} \odot \mu^{\mathbf{t}} &\neq e^{i\theta_{\mathbf{t}}} f^{\mathbf{t}} \odot \mu^{\mathbf{t}} \end{aligned}$$

even when the mask estimate is perfectly accurate.

Mask phase constraint (MPC)

- Let μ^0 be a nonvanishing random mask with phase at each pixel continuously and independently distributed according to a nonvanishing probability density function p_γ on $(-\gamma\pi, \gamma\pi]$ with a constant $\gamma \leq 1$.
- Suppose our mask estimate is ν^0. Write the relative mask error as

$$\alpha(\mathbf{n}) \exp[i\phi(\mathbf{n})] = \nu^0(\mathbf{n})/\mu^0(\mathbf{n}), \quad \alpha(\mathbf{n}) > 0.$$

- F. & Chen (2018): ν^0 *satisfies MPC if*

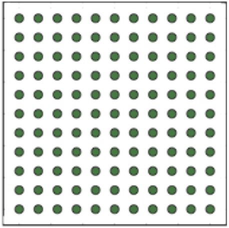
$$|\phi(\mathbf{n}) - \phi_0| < \min\{\gamma, 1/2\} \quad \mod 2\pi,$$

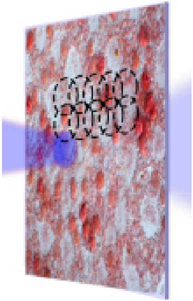
for a constant ϕ_0, *i.e.* $\nu^0(\mathbf{n})$ *is pointing in the half plane in* $\mathbb{C}$ *with the normal vector* $\mu^0(\mathbf{n})$ *for all* $\mathbf{n}$.

Counter-examples exist!

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.





Block phase

Theorem (F 2018)

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

$$\nu^k(\mathbf{n})g^k(\mathbf{n}) = e^{\mathrm{i}\theta_k}\mu^k(\mathbf{n})f^k(\mathbf{n}), \quad \text{for all } \mathbf{n} \in \mathcal{M}^k \text{ and } \mathbf{t}_k \in \mathcal{T}.$$

If

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

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

Non-APA ambiguity

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

$$f = \begin{bmatrix} f_{00} & f_{10} & f_{20} \\ f_{01} & f_{11} & f_{21} \\ f_{02} & f_{12} & f_{22} \end{bmatrix}, \quad g = \begin{bmatrix} f_{00} & e^{\mathrm{i}2\pi/3} f_{10} & e^{\mathrm{i}4\pi/3} f_{20} \\ e^{\mathrm{i}2\pi/3} f_{01} & e^{\mathrm{i}4\pi/3} f_{11} & f_{21} \\ e^{\mathrm{i}4\pi/3} f_{02} & f_{12} & e^{\mathrm{i}2\pi/3} f_{22} \end{bmatrix}$$

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

$$\mu^{kl} = \begin{bmatrix} \mu^{kl}_{00} & \mu^{kl}_{10} \\ \mu^{kl}_{01} & \mu^{kl}_{11} \end{bmatrix}, \quad \nu^{kl} = \begin{bmatrix} \mu^{kl}_{00} & e^{-\mathrm{i}2\pi/3} \mu^{kl}_{10} \\ e^{-\mathrm{i}2\pi/3} \mu^{kl}_{01} & e^{-\mathrm{i}4\pi/3} \mu^{kl}_{11} \end{bmatrix}, \quad k, l = 0, 1, 2,$$

be the probe and its estimate, respectively, where $\mu^{kl}_{ij}, \nu^{kl}_{ij} \in \mathbb{C}^{n/3 \times n/3}$.
It is verified straightforwardly that $\nu^{ij} \odot g^{ij} = e^{\mathrm{i}(i+j)2\pi/3} \mu^{ij} \odot f^{ij}$.

Periodic ambiguity (raster grid pathology)

$(\tau = m/2)$ $\mathbf{t}_{kl}$-shifted probes μ^{kl} and ν^{kl} can be written as

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

Let

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

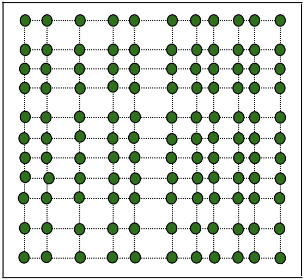
Consider the two objects

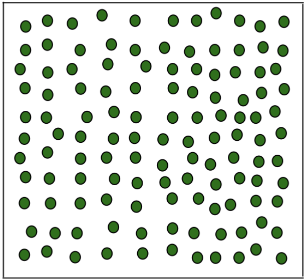
$$f = \begin{bmatrix} f_{00} & \cdots & f_{q-1,0} \\ \vdots & \vdots & \vdots \\ f_{0,q-1} & \cdots & f_{q-1,q-1} \end{bmatrix}, \quad g = \left[\epsilon^{-1} \odot f_{ij}\right]$$

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

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 $\mathrm{gcd}_{j_k}\{|a_{j_k}^i|\} = 1, \quad i = 1, 2,$ *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 $\mathbf{r}$

$$\begin{aligned} g(\mathbf{n})/f(\mathbf{n}) &= \alpha^{-1}(0)\exp(\mathrm{i}\mathbf{n}\cdot\mathbf{r}), \\ \nu^0(\mathbf{n})/\mu^0(\mathbf{n}) &= \alpha(0)\exp(\mathrm{i}\phi(0) - \mathrm{i}\mathbf{n}\cdot\mathbf{r}) \\ \theta_{kl} &= \theta_{00} + \mathbf{t}_{kl}\cdot\mathbf{r}. \end{aligned}$$

Mixing schemes

Theorem (F & Chen 2018)

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

$$\begin{aligned} g(\mathbf{n})/f(\mathbf{n}) &= \alpha^{-1}(0)\exp(\mathrm{i}\mathbf{n}\cdot\mathbf{r}), \\ \nu^0(\mathbf{n})/\mu^0(\mathbf{n}) &= \alpha(0)\exp(\mathrm{i}\phi(0) - \mathrm{i}\mathbf{n}\cdot\mathbf{r}) \\ \theta_{\mathbf{t}} &= \theta_0 + \mathbf{t}\cdot\mathbf{r}. \end{aligned}$$

Alternating minimization

$|\mathcal{F}(\mu, f)| = b$: the ptychographic data. Define $A_k h := \mathcal{F}(\mu_k, h)$, $B_k \eta := \mathcal{F}(\eta, f_{k+1})$. We have $A_k f_{j+1} = B_j \mu_k$.

1. Initial guess μ_1.
2. Update the object estimate $\quad f_{k+1} = \underset{g \in \mathbb{C}^{n\times n}}{\operatorname{argmin}} \mathcal{L}(A_k^* g)$
3. Update the probe estimate $\quad \mu_{k+1} = \underset{\nu \in \mathbb{C}^{m\times m}}{\operatorname{argmin}} \mathcal{L}(B_k^* \nu)$
4. Terminate when $\| |B_k^* \mu_{k+1}| - b \|$ is less than tolerance or stagnates. If not, go back to step 2 with $k \to k+1$.

Two non-convex log-likelihood functions:

$$\begin{aligned} \text{Poisson:} \quad \mathcal{L}(y) &= \sum_i |y[i]|^2 - b^2[i] \ln |y[i]|^2 \\ \text{Gaussian:} \quad \mathcal{L}(y) &= \frac{1}{2} \| |y| - b \|^2. \end{aligned}$$

The Gaussian is non-differentiable and the hight SNR and near critical limit of the Poisson.

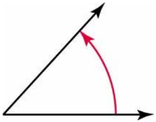
Initialization

- Mask/probe initialization

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

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

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



Relative error of the mask estimate

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

- Object initialization: $f_1 =$ constant or random phase object.

Douglas-Rachford splitting (DRS)

Each minimization can be cast into the form:

$$\arg \min_{g \in \mathbb{C}^{n\times n}} \mathcal{L}(A_k^* g) \Longrightarrow \arg \min_u K(u) + \mathcal{L}(u)$$

where

$$K = \text{Indicator function of} \quad \{A_k^* x : x \in \mathbb{C}^{n\times n}\}.$$

DRS is defined by the following iteration for $l = 1, 2, 3 \cdots$

$$\begin{aligned} y^{l+1} &= \text{prox}_{K/\rho}(u^l); \\ z^{l+1} &= \text{prox}_{\mathcal{L}/\rho}(2y^{l+1} - u^l) \\ u^{l+1} &= u^l + z^{l+1} - y^{l+1} \end{aligned}$$

where

$$\begin{aligned} \text{prox}_{K/\rho}(u) &= A_k^*(A_k^*)^\dagger u \\ \text{prox}_{\mathcal{L}/\rho}(u) &= \operatorname*{argmin}_x \mathcal{L}(x) + \frac{\rho}{2}\|x - u\|^2. \end{aligned}$$

Fixed point algorithm with Gaussian log-likelihood

- $\rho = 1$
- Reflectors: $R_k = 2P_k - I, S_k = 2Q_k - I$.
- Gaussian:

$$
\begin{aligned}
u_k^{l+1} &= \frac{1}{2}u_k^l + \frac{1}{2}b \odot \mathrm{sgn}\left(R_k u_k^l\right) \\
v_k^{l+1} &= \frac{1}{2}v_k^l + \frac{1}{2}b \odot \mathrm{sgn}\left(S_k v_k^l\right).
\end{aligned}
$$

- Poisson:

$$
\begin{aligned}
u_k^{l+1} &= \frac{1}{2}u_k^l - \frac{1}{3}R_k u_k^l + \frac{1}{6}\sqrt{|R_k u_k^l|^2 + 24b^2} \odot \mathrm{sgn}\left(R_k u_k^l\right) \\
v_k^{l+1} &= \frac{1}{2}v_k^l - \frac{1}{3}S_k v_k^l + \frac{1}{6}\sqrt{|S_k v_k^l|^2 + 24b^2} \odot \mathrm{sgn}\left(S_k v_k^l\right).
\end{aligned}
$$

Fixed-point analysis

Proposition

Let $\rho \geq 1$. Let (u, v) be a linearly stable fixed point. Then $f_\infty := A_\infty^\dagger u$ and $\mu_\infty := B_\infty^\dagger v$ are a solution to blind ptychography, i.e. $|\mathcal{F}(\mu_\infty, f_\infty)| = b$.

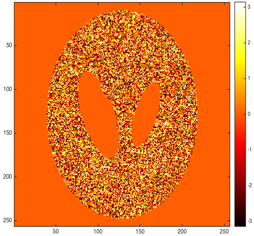
Proposition

Let (u, v) be the true solution. Then $\|J_A(\eta)\|_2 \leq \|\eta\|_2, \|J_B(\xi)\|_2 \leq \|\xi\|_2$ for all $\eta, \xi \in \mathbb{C}^N$ and the equality holds in the direction $\pm \imath b/\|b\|$ (and possibly elsewhere on the unit sphere).

Test objects and error metric

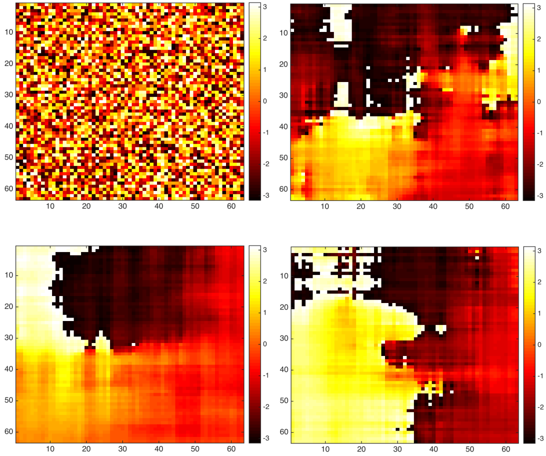
$+\quad \imath$

$\times \exp \imath$



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

Masks

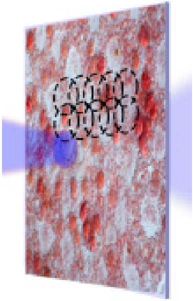


correlation length $c = 0, 0.4m, 0.7m, 1m$

Scanning schemes

- 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)



Dark-field vs. periodic BC

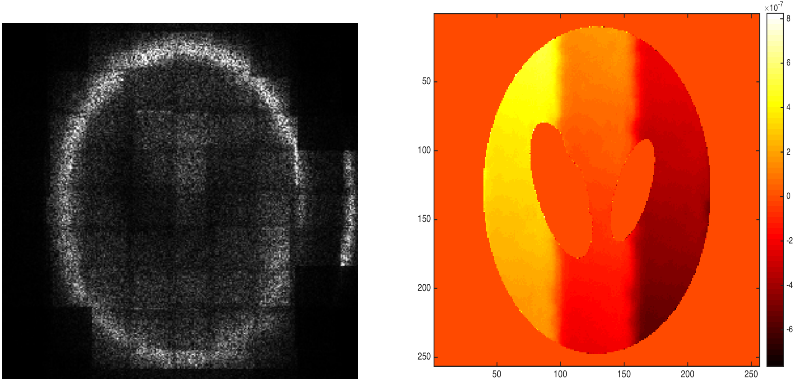
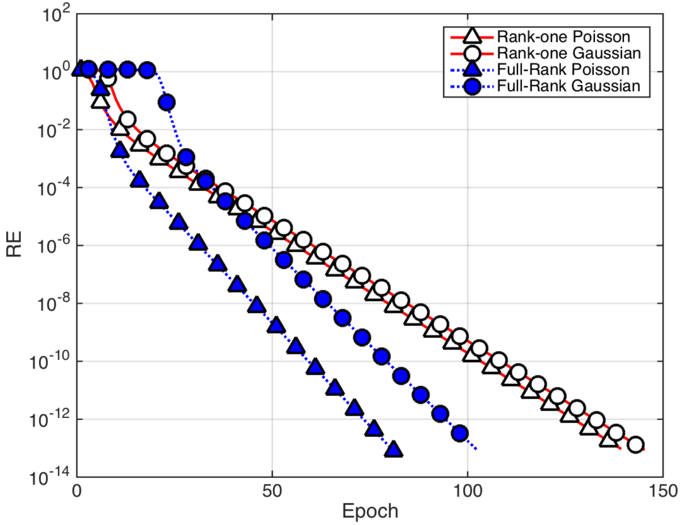
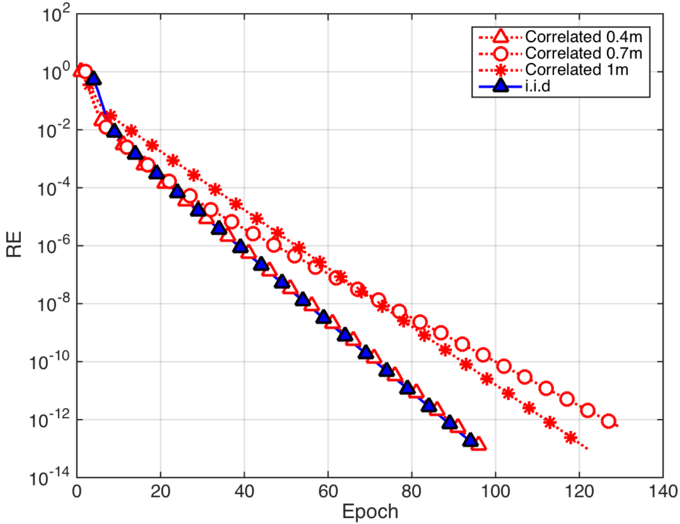


Figure: (Left) Reconstructed moduli with dark-field BC & 30 inner iterations; (right) Reconstructed phase error with periodic BC & 80 inner iterations

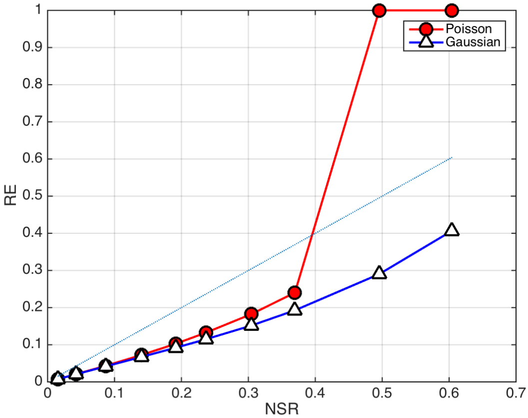
Experiment: Rank-one vs. full-rank



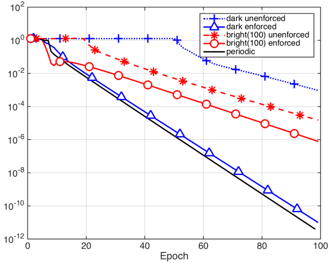
Experiment: Independent vs. correlated mask



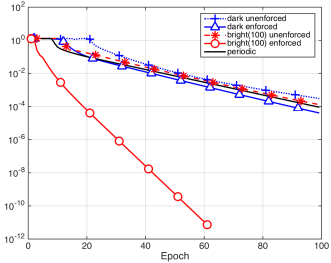
Noise robustness



Boundary conditions



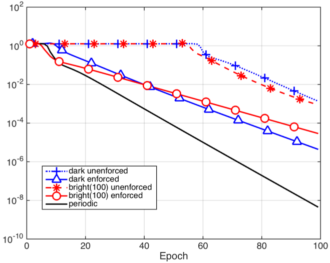
(a) CiB with PPC(0, 0, 0.5)



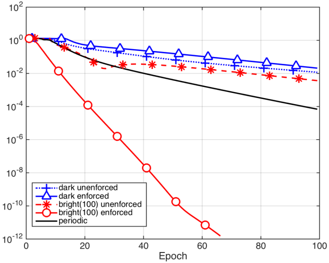
(b) RPP with PPC(0, 0, 0.4)

Full-rank scheme

Boundary conditions



(c) CiB with PPC(0, 0, 0.5)

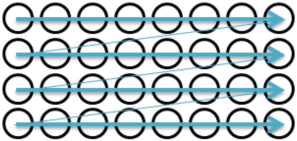


(d) RPP with PPC(0, 0, 0.4)

Rank-1 scheme

Conclusion

1. **Theory**: blind ptychography can recover simultaneously the object and the probe/mask up to an affine phase factor and a constant amplitude offset.
   - → Mixing schemes
   - → Raster scan pathology
2. **Algorithm**: MPC Initialization + AMDRS (Convergence proof?)
3. Position uncertainty ?



References

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Thank you!