Holographic Phase Retrieval and Optimal Reference Design

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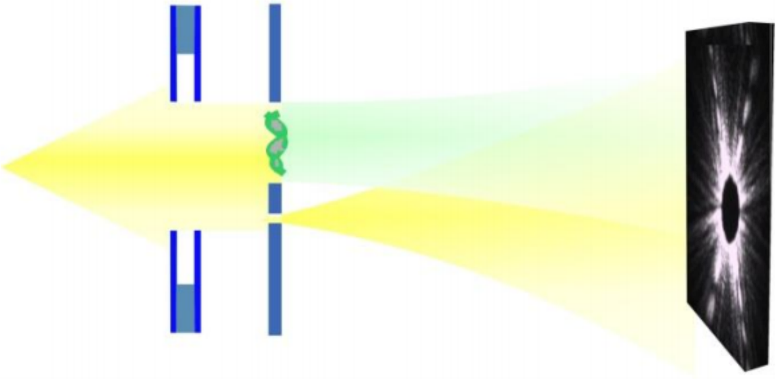
The Phase Retrieval Problem

Given $\left|\widehat{X}(\omega)\right|^2 \doteq \left|\int_{t\in T} X(t)e^{-i\omega t}\right|^2, \quad \omega \in \Omega,$

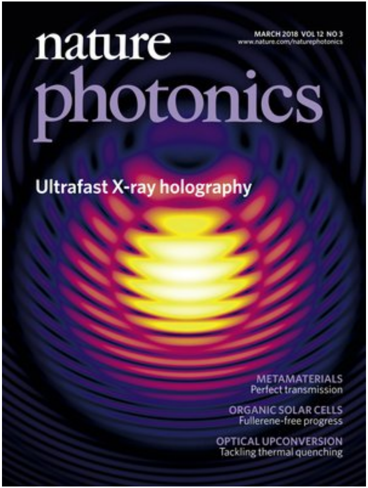
Recover $X.$

Coherent Diffraction Imaging (CDI)

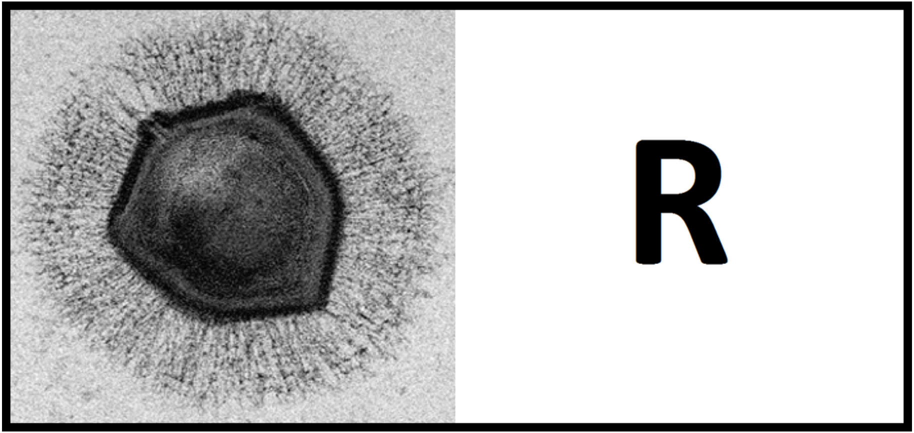
Holographic CDI



Holographic CDI



Specimen and Reference Setup



Popular Reference Choices

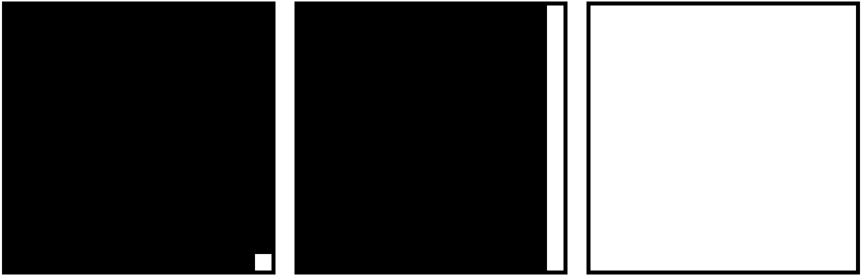


Figure: Pinhole, Slit, and Block references.

The Holographic Phase Retrieval Problem

Given $R \in \mathbb{R}^{n \times n}, \quad \left|\widehat{[X, R]}\right|^2 \in \mathbb{R}^{m \times m},$

Recover $X \in \mathbb{R}^{n \times n}.$

The Holographic Phase Retrieval Problem

$$\textbf{Given} \quad R \in \mathbb{R}^{n\times n}, \quad \left|\widehat{[X,R]}\right|^2 \in \mathbb{R}^{m\times m},$$
$$\textbf{Recover} \quad X \in \mathbb{R}^{n\times n}.$$

Knowing R makes a huge difference!

Exact Recovery for Noiseless Data

Step 1: Transform to the time domain $A_{[X,R]} = \mathcal{F}^{-1}\left(\left|\widehat{[X,R]}\right|^2\right)$.

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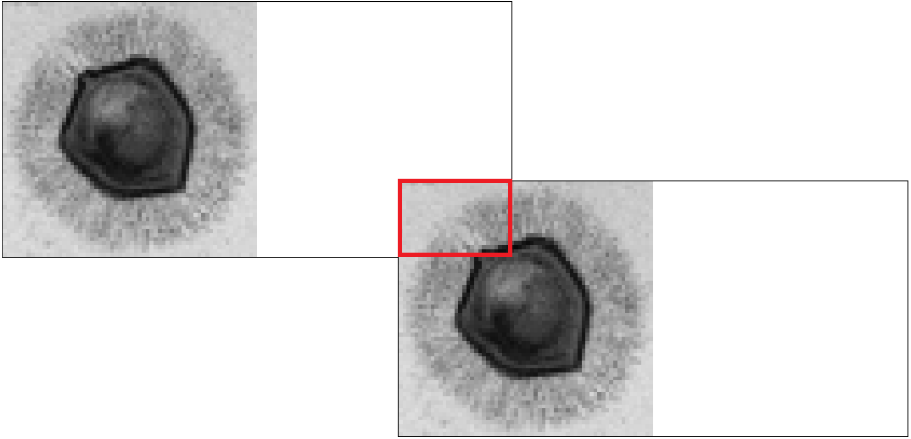
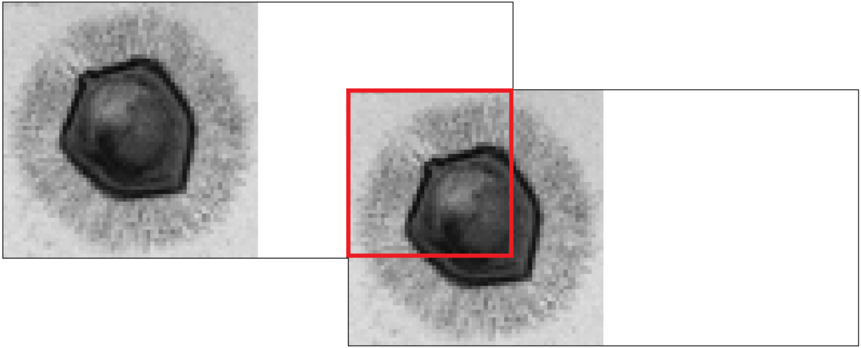
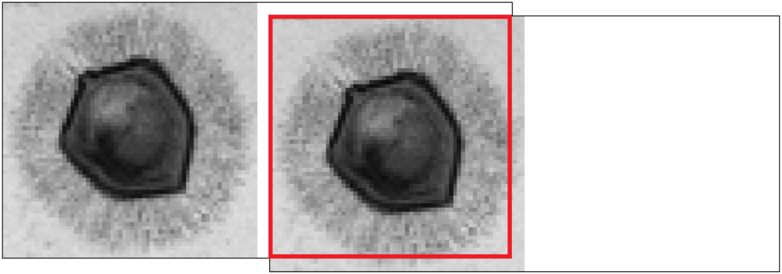


Exact Recovery for Noiseless Measurements





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Step 1: Transform to the time domain $A_{[X,R]} = \mathcal{F}^{-1}\left(\left|\widehat{[X,R]}\right|^2\right)$.

Step 2: Extract $C^{\diamond}_{[X,R]}$, the top-left quadrant of $A_{[X,R]}$. This is one quadrant of the cross-correlation of X and R.

Step 3: De-convolve R and X.

$$\mathrm{vec}(X) = M_R^{-1}\,\mathrm{vec}(C_{[X,R]}).$$

For

$$R = \begin{bmatrix} r_{00} & r_{01} & r_{02} \\ r_{10} & r_{11} & r_{12} \\ r_{20} & r_{21} & r_{22} \end{bmatrix},$$

$$M_R = \left[\begin{array}{ccc|ccc|ccc} r_{22} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ r_{12} & r_{22} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ r_{02} & r_{12} & r_{22} & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline r_{21} & 0 & 0 & r_{22} & 0 & 0 & 0 & 0 & 0 \\ r_{11} & r_{21} & 0 & r_{12} & r_{22} & 0 & 0 & 0 & 0 \\ r_{01} & r_{11} & r_{21} & r_{02} & r_{12} & r_{22} & 0 & 0 & 0 \\ \hline r_{20} & 0 & 0 & r_{21} & 0 & 0 & r_{22} & 0 & 0 \\ r_{10} & r_{20} & 0 & r_{11} & r_{21} & 0 & r_{12} & r_{22} & 0 \\ r_{00} & r_{10} & r_{20} & r_{01} & r_{11} & r_{21} & r_{02} & r_{12} & r_{22} \end{array}\right].$$

Altogether, this gives a linear relationship between $\left|\widehat{[X, R]}\right|^2$ and X !

$$\mathrm{vec}(X) = T_R \,\mathrm{vec}\left(\left|\widehat{[X, R]}\right|^2\right).$$

Noisy Data

Given $Y^\star$, a possibly noise-corrupted version of $Y = |\widehat{[X, R]}|^2$, this procedure, – the **Referenced Deconvolution Algorithm** – gives $X^\star$, the solution of

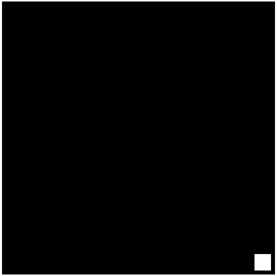
$$\min_X \frac{1}{2} \left\| Y^\star - \left|\widehat{[X, R]}\right|^2 \right\|^2.$$

Special Cases

For popular reference choices, M_R has a special structure that is fast to invert!

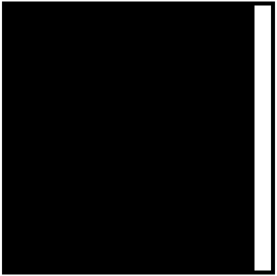
This places within a broader context various reference-specific algorithms.

Pinhole Reference



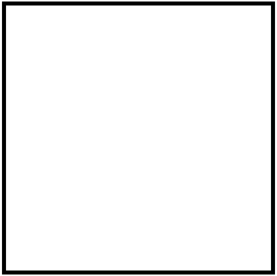
$$M_R = I_{n^2}.$$

Slit Reference



$M_R = I_n \otimes D_n$, where D_n is the *difference matrix* (1's on diagonal, -1's on first subdiagonal).

Block Reference



$$M_R = D_n \otimes D_n.$$

Error Formula

Since $\mathrm{vec}(X) = T_R \, \mathrm{vec}(Y)$ and $\mathrm{vec}(X^\star) = T_R \, \mathrm{vec}(Y^\star)$,

$$\begin{aligned} &\mathbb{E}\|X^\star - X\|_F^2 \\ &= \left\langle T_R^* T_R, \mathbb{E}\Big(\mathrm{vec}(Y^\star) - \mathrm{vec}(Y)\Big)\Big(\mathrm{vec}(Y^\star) - \mathrm{vec}(Y)\Big)^* \right\rangle_F . \end{aligned}$$

Poisson shot noise model

Quantum mechanics $\rightarrow$ # of photons emitted by an X-ray source is random (Poisson process)

Np: total # of photons emitted

$$\widehat{Y} \sim_{\text{ind}} \frac{\|Y\|_1}{N_p} \text{Pois}\left(\frac{N_p}{\|Y\|_1} Y\right),$$

Poisson noise error formula

$$\mathbb{E}\|X^\star - X\|_F^2 = \left\langle T_R^* T_R, \frac{\|Y\|_1}{N_p} \operatorname{diag}(\operatorname{vec}(Y)) \right\rangle_F$$
$$= \left\langle S_R, \frac{\|Y\|_1}{N_p} Y \right\rangle_F,$$

where $S_R = \operatorname{reshape}\Big(\operatorname{diag}(T_R^* T_R), m, m \Big)$.

Poisson noise error formula

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$$= \left\langle S_R, \frac{\|Y\|_1}{N_p} Y \right\rangle_F,$$

where $S_R = \operatorname{reshape}\Big(\operatorname{diag}(T_R^* T_R), m, m \Big)$.

$\rightarrow$ each frequency $Y(k_1, k_2)$ is scaled by $S_R(k_1, k_2)$.

Computationally inefficient to compute $T_R^* T_R$ just to extract its diagonal.

Theorem

$$\mathbb{E}\|X^\star - X\|_F^2 = \text{vec}((M_R^{-1})^T)^T W_Y \, \text{vec}((M_R^{-1})^T),$$

where

$$W_Y = I_{n^2} \otimes \left(\sum_{k_1,k_2=0}^{m-1} \frac{\|Y\|_1}{N_P} Y(k_1, k_2) W_{k_1,k_2} \right),$$

and $W_{k_1,k_2} \in \mathbb{R}^{n^2 \times n^2}$ *is given by*
$W_{k_1,k_2}(p, q) = \exp\left(\frac{2\pi i}{m}(k_1(p_1 - q_1) + k_2(p_2 - q_2)) \right)$ *for*
$p_1, p_2, q_1, q_2 \in \{0, \ldots, n-1\}$, $p = np_1 + p_2$ *and* $p = np_1 + p_2$.

Uniform Lower Bound on $S_R(k_1, k_2)$

Theorem

For any reference R and all $k_1, k_2 \in \{0, \dots, m-1\}$,

$$S_R(k_1, k_2) \geq \frac{1}{m^4}.$$

Pinhole Reference

Theorem

For the pinhole reference R_p and $k_1, k_2 \in \{0, \ldots, m-1\}$,

$$S_{R_p}(k_1, k_2) = \frac{n^2}{m^4}.$$

Slit Reference

Theorem

For the slit reference R_s and $k_1, k_2 \in \{0, \ldots, m-1\}$,

$$S_{R_s}(k_1, k_2) = \frac{n}{m^2}\left(\frac{1}{m^2} + \frac{2(n-1)}{m^2}\Big(1 - \cos(\frac{2\pi k_2}{m})\Big)\right).$$

Block Reference

Theorem

For the block reference R_b and $k_1, k_2 \in \{0, \ldots, m-1\}$,

$$S_{R_b}(k_1, k_2) =$$

$$\left(\frac{1}{m^2} + \frac{2(n-1)}{m^2}\Big(1 - \cos(\frac{2\pi k_1}{m})\Big)\right)\left(\frac{1}{m^2} + \frac{2(n-1)}{m^2}\Big(1 - \cos(\frac{2\pi k_2}{m})\Big)\right).$$

So which is the best reference choice?

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$\rightarrow$ Depends on the frequency distribution of Y.

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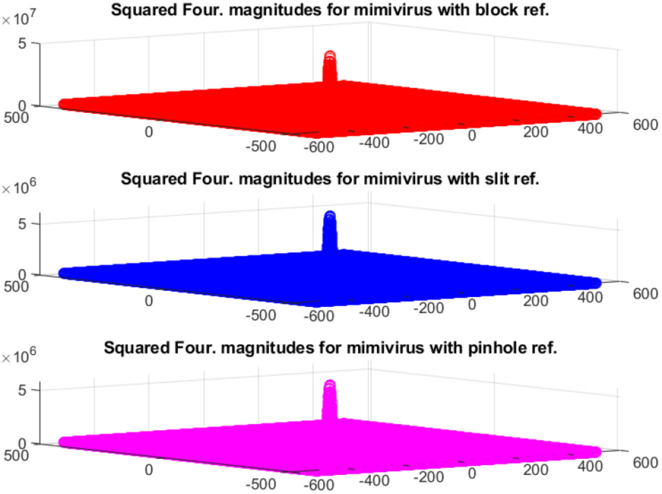
→ Depends on the frequency distribution of Y.

Typically, Y has a rapidly decaying shape.

Mimivirus Spectrum Squared Magnitudes



Block Reference Optimality

For a decaying frequency specimen, the block reference provides the best error scaling of the three popular choices.
It is also optimal or near-optimal amongst all possible references.

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It is also optimal or near-optimal amongst all possible references.

Theorem

For the block reference R_b, $S_{R_b}(k_1, k_2)$ deviates from the uniform lower bound on $S_R(k_1, k_2)$ at a rate of

$$\frac{2n}{m^2} \max\left(1 - \cos(\frac{2\pi k_1}{m}), 1 - \cos(\frac{2\pi k_2}{m})\right). \tag{3.1}$$

So, when $(k_1, k_2) = (0, 0)$, the block reference achieves the lower error bound, and for small k_1, k_2 deviates by a small numerical factor.

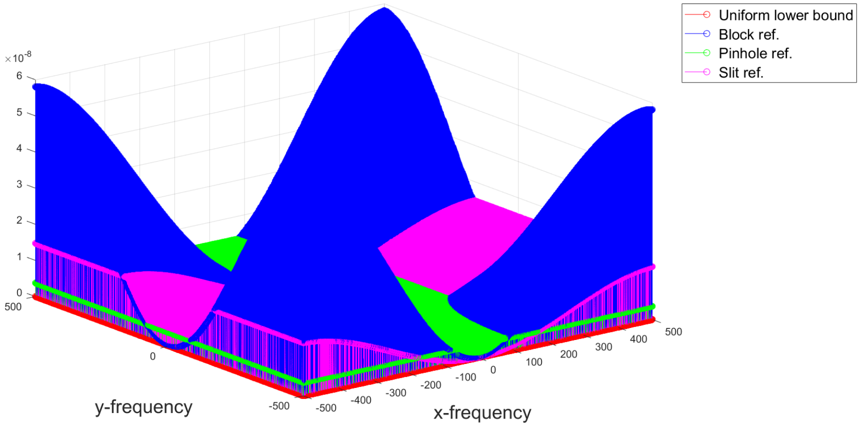
Flat Spectrum Images - Pinhole Reference Optimality

Theorem

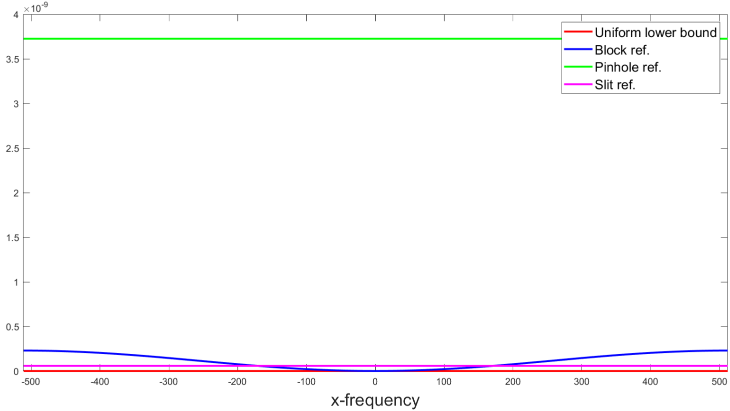
The pinhole reference R_p is the unique reference choice which provides a constant scaling to all frequencies.

So, the pinhole reference is ideal for “flat-spectrum” images.

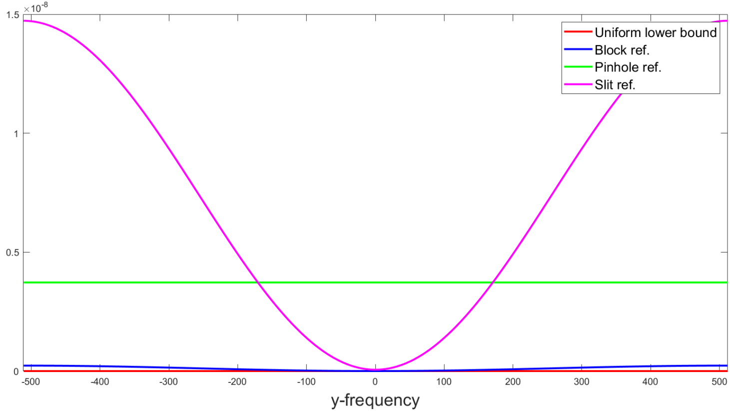
Frequency Scaling Comparison



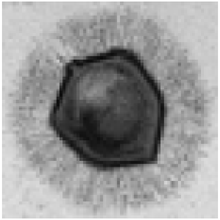
Frequency Scaling Comparison



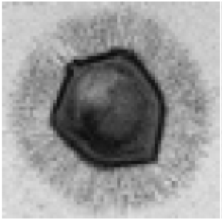
Frequency Scaling Comparison



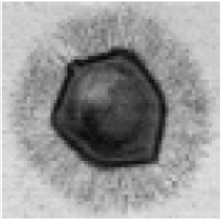
Decaying Spectrum Image (Typical)



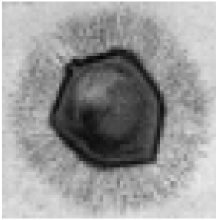
(a) Ground-truth image
(No Exp. Err.)
(No Theory Err.)



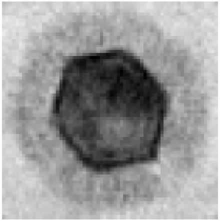
(b) Ref. Deconv. with block ref.
Exp. Err. = 0.0202
Theory Err. = 0.0195



(c) Ref. Deconv. with slit ref.
Exp. Err. = 0.0277
Theory Err. = 0.0227

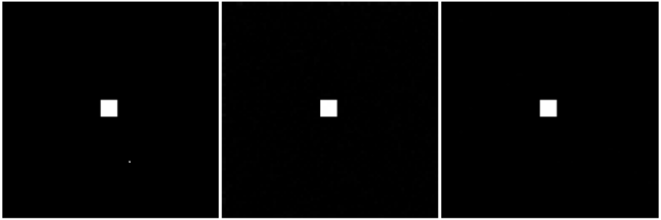


(d) Ref. Deconv. with pinhole ref.
Exp. Err. = 0.0606
Theory Err. = 0.0799



(h) HIO (no ref.)
Exp. Err. = 0.1474
Theory Err. N/A

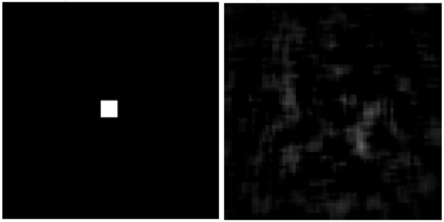
Flat Spectrum Image



(a) Ground-truth image
(No Exp. Err.)
(No Theory Err.)

(b) Ref. Deconv. with block ref.
Exp. Err. = 0.0955
Theory Err. = 0.0915

(c) Ref. Deconv. with slit ref.
Exp. Err. = 0.0137
Theory Err. = 0.0136



(d) Ref. Deconv. with pinhole ref.
Exp. Err. = 0.0103
Theory Err. = 0.0103

(h) HIO (no ref.)
Exp. Err. = 1.4689
Theory Err. N/A

Thank you!