Holographic Phase Retrieval and Optimal Reference Design

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December 6, 2018
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Table of Contents

1 The Holographic Phase Retrieval Problem

2 Referenced Deconvolution Algorithm

3 Error Analysis and Optimal Reference Design

4 Numerical Experiments
The Phase Retrieval Problem

Given \[ |\hat{X}(\omega)|^2 = \left| \int_{t \in T} X(t)e^{-i\omega t} \right|^2, \quad \omega \in \Omega, \]

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 \( R \in \mathbb{R}^{n \times n} \), \( \left| \widehat{[X, R]} \right|^2 \in \mathbb{R}^{m \times m} \),

Recover \( X \in \mathbb{R}^{n \times n} \).
The Holographic Phase Retrieval Problem

Given $R \in \mathbb{R}^{n \times n}$, $\|X, R\|^2 \in \mathbb{R}^{m \times m}$,

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

Knowing $R$ makes a huge difference!
Exact Recovery for Noiseless Data

Step 1: Transform to the time domain $A_{[X,R]} = \mathcal{F}^{-1}(\|\hat{X,R}\|^2)$. 
Exact Recovery for Noiseless Data

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

Step 2: Extract $C_{[X,R]}$, the top-left quadrant of $A_{[X,R]}$. 
Exact Recovery for Noiseless Data

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

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

Exact Recovery for Noiseless Measurements
Exact Recovery for Noiseless Data

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

Step 2: Extract $C_{[X,R]}$, the top-left quadrant of $A_{[X,R]}$. 
Exact Recovery for Noiseless Data

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

Step 2: Extract $C_{[X,R]}$, 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 $X$.

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

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

\[
M_R = \begin{bmatrix}
  r_{22} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
  r_{12} & r_{22} & 0 & 0 & 0 & 0 & 0 & 0 \\
  r_{02} & r_{12} & r_{22} & 0 & 0 & 0 & 0 & 0 \\
  r_{21} & 0 & 0 & r_{22} & 0 & 0 & 0 & 0 \\
  r_{11} & r_{21} & 0 & r_{12} & r_{22} & 0 & 0 & 0 \\
  r_{01} & r_{11} & r_{21} & r_{02} & r_{12} & r_{22} & 0 & 0 \\
  r_{20} & 0 & 0 & r_{21} & 0 & 0 & r_{22} & 0 \\
  r_{10} & r_{20} & 0 & r_{11} & r_{21} & 0 & r_{12} & r_{22} \\
  r_{00} & r_{10} & r_{20} & r_{01} & r_{11} & r_{21} & r_{02} & r_{12} & r_{22}
\end{bmatrix}.
\]
Altogether, this gives a linear relationship between $|[\hat{X}, R]|^2$ and $X!$

$$\text{vec}(X) = T_R \text{vec} \left( |[\hat{X}, R]|^2 \right).$$
Noisy Data

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

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

\[ M_R = I_n^2. \]
$M_R = I_n \otimes D_n$, where $D_n$ is the difference matrix (1’s on diagonal, -1’s on first subdiagonal).
$M_R = D_n \otimes D_n$. 
Error Formula

Since \( \text{vec}(X) = T_R \text{vec}(Y) \) and \( \text{vec}(X^*) = T_R \text{vec}(Y^*) \),

\[
\mathbb{E} \| X^* - X \|_F^2 = \left\langle T_R^* T_R, \mathbb{E} \left( \text{vec}(Y^*) - \text{vec}(Y) \right) \left( \text{vec}(Y^*) - \text{vec}(Y) \right)^* \right\rangle_F.
\]
Poisson shot noise model

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

$N_p$: total # of photons emitted

$$\hat{Y} \sim_{\text{ind}} \frac{1}{N_p} \text{Pois}\left(\frac{N_p}{\|Y\|_1} Y\right),$$
Poisson noise error formula

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

where \( S_R = \text{reshape} \left( \text{diag} \left( T_R^* T_R \right), m, m \right) \).
Poisson noise error formula

\[ \mathbb{E}\|X^* - X\|_F^2 = \left\langle T_R^* T_R, \frac{\|Y\|_1}{N_p} \text{diag}(\text{vec}(Y)) \right\rangle_F \]

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

where \( S_R = \text{reshape}\left(\text{diag}(T_R^* T_R), m, m\right) \).

→ 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**

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

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 $k_1, k_2 \in \{0, \ldots, m - 1\}$,*

\[ S_R(k_1, k_2) \geq \frac{1}{m^4}. \]
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 $k_1, k_2 \in \{0, \ldots, m - 1\}$,

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

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

\[ S_{R_b}(k_1, k_2) = \left(\frac{1}{m^2} + \frac{2(n - 1)}{m^2} \left(1 - \cos\left(\frac{2\pi k_1}{m}\right)\right)\right) \left(\frac{1}{m^2} + \frac{2(n - 1)}{m^2} \left(1 - \cos\left(\frac{2\pi k_2}{m}\right)\right)\right). \]
So which is the best reference choice?
So which is the best reference choice?

→ Depends on the frequency distribution of $Y$. 
So which is the best reference choice?
→ Depends on the frequency distribution of $Y$.
Typically, $Y$ has a rapidly decaying shape.
Mimivirus Spectrum Squared Magnitudes

Squared Four. magnitudes for mimivirus with block ref.

Squared Four. magnitudes for mimivirus with slit ref.

Squared Four. magnitudes for mimivirus with pinhole ref.
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.
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.

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

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

(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

- Uniform lower bound
- Block ref.
- Pinhole ref.
- Slit ref.
Frequency Scaling Comparison

![Graph showing frequency scaling comparison with different reference designs. The graph plots frequency (x-frequency) against a value on the y-axis. Legend includes Uniform lower bound, Block ref., Pinhole ref., and Slit ref., with the latter two showing minimal deviation from the lower bound.]
Decaying Spectrum Image (Typical)
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!