Holographic Phase Retrieval and Dual-Reference Design

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Collaborators

- Dr. Ju Sun
- Prof. Emmanuel Candès
- Dr. T.J. Lane
- Po-Nan Li

Papers

- **Holographic Phase Retrieval and Optimal Reference Design**
  David A. Barmherzig, Ju Sun, Emmanuel J. Candès, T.J. Lane, and Po-Nan Li.
  Submitted to Inverse Problems, 2018.
  `arxiv.org/abs/1901.06453`
- **Dual-Reference Design for Holographic Coherent Diffraction Imaging**
  David A. Barmherzig, Ju Sun, Emmanuel J. Candès, T.J. Lane, and Po-Nan Li.
  Submitted to SampTA, 2019.
  `arxiv.org/abs/1902.02492`
- Available at `davidbar.org/publications`

Table of Contents

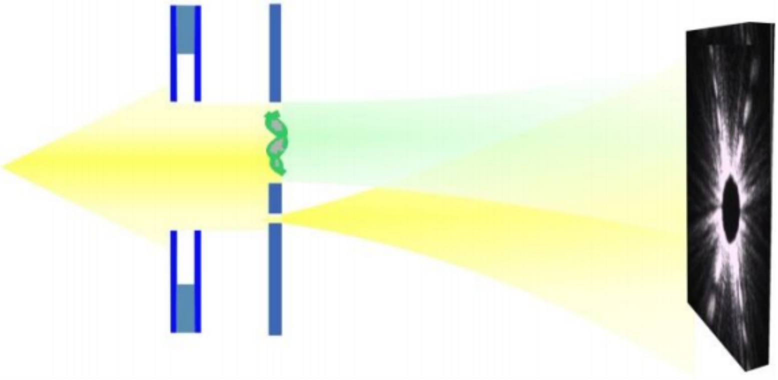
The Phase Retrieval Problem

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

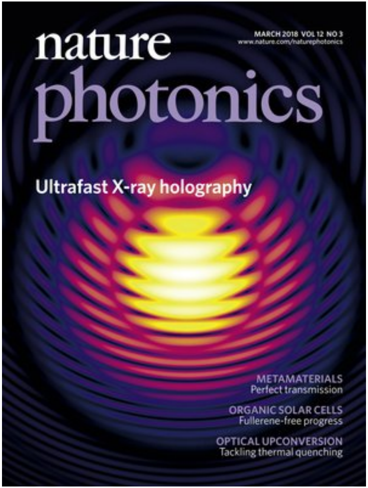
Recover X.

Coherent Diffraction Imaging (CDI)

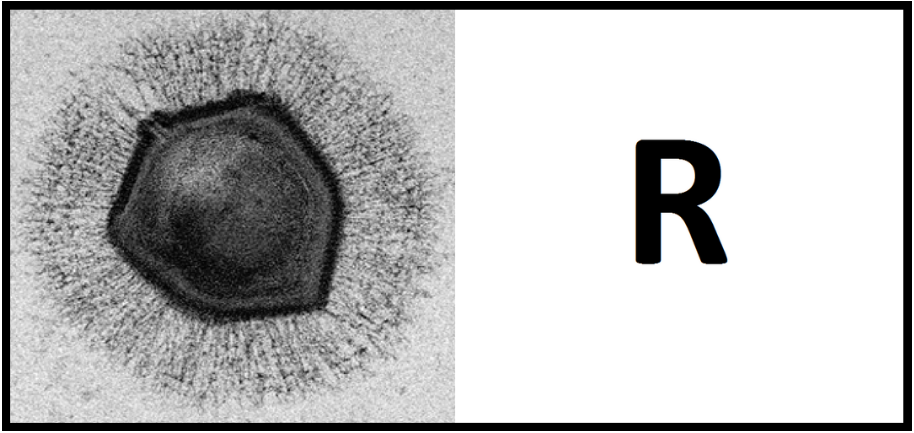
Holographic CDI



Holographic CDI



Specimen and Reference Setup



Popular Reference Choices

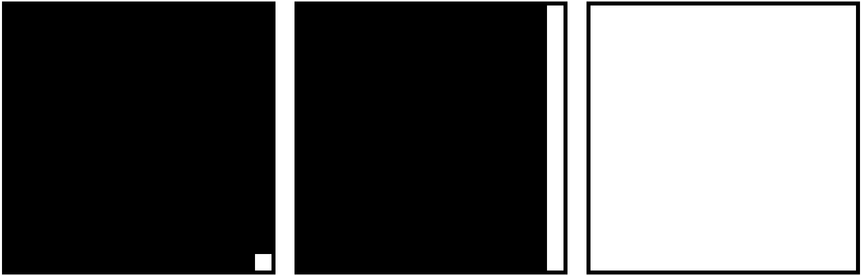


Figure: Pinhole, Slit, and Block references.

The Holographic Phase Retrieval Problem

Given $R \in \mathbb{R}^{n\times n}, \quad Y = \left|\mathcal{F}([X, R])\right|^2 \in \mathbb{R}^{m\times m},$

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

The Holographic Phase Retrieval Problem

Given $R \in \mathbb{R}^{n\times n}, \quad Y = \left|\mathcal{F}([X, R])\right|^2 \in \mathbb{R}^{m\times m},$
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 $A_{[X,R]} = \mathcal{F}^{-1}(Y)$.

Exact Recovery for Noiseless Data

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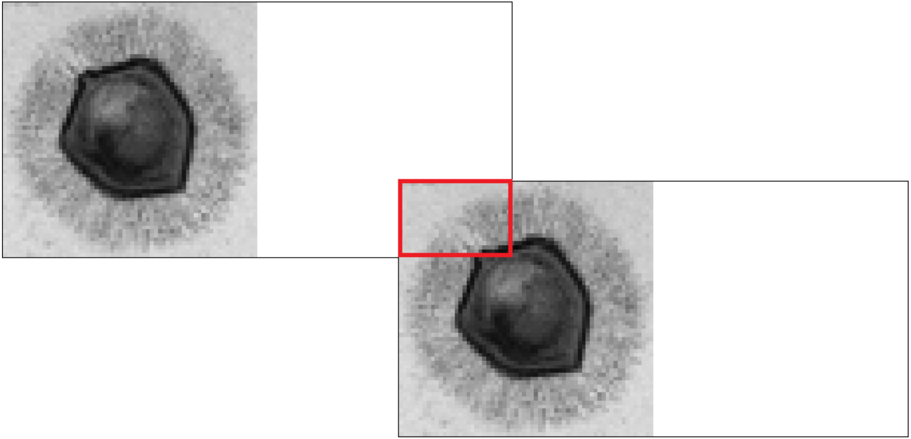
Step 2: Extract $C^{\diamond}_{[X,R]}$, the top-left quadrant of $A_{[X,R]}$.

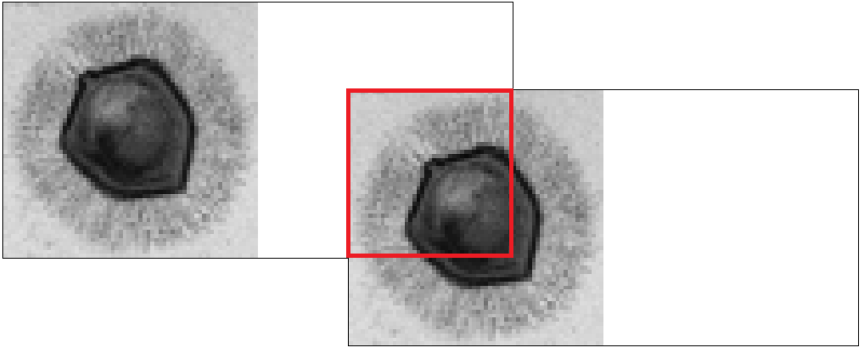
Exact Recovery for Noiseless Data

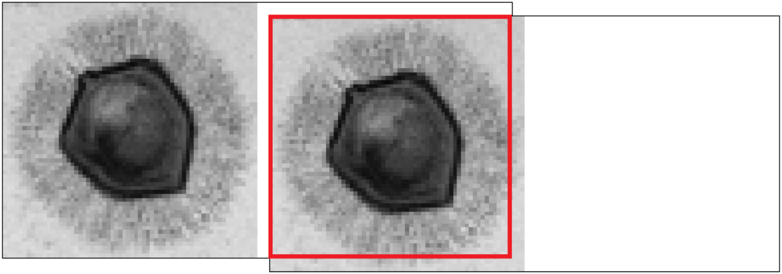
Step 1: Transform to the time domain $A_{[X,R]} = \mathcal{F}^{-1}\big(Y\big)$.

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.



Exact Recovery for Noiseless Measurements





Exact Recovery for Noiseless Data

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

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.

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

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

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 Y and X !

$$\mathrm{vec}(X) = T_R \, \mathrm{vec}\left(Y\right).$$

Noisy Data

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

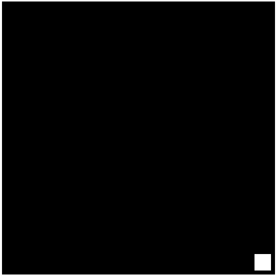
$$\min_X \frac{1}{2}\left\|Y^\star - \left|\mathcal{F}([X, R])\right|^2\right\|^2.$$

Special Cases

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

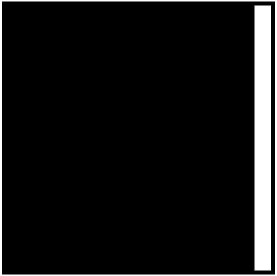
This places within a broader context various reference-specific algorithms.

Pinhole Reference



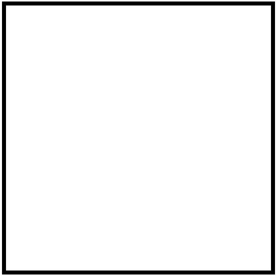
$$M_R = I_{n^2}.$$

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 reaching detector

$$\hat{Y} \sim_{\text{ind}} \frac{\|Y\|_1}{N_p} \text{Pois}\Big(\frac{N_p}{\|Y\|_1} Y\Big),$$

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

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

$\rightarrow$ each frequency $Y(k_1, k_2)$ is scaled by the **reference scaling factor** S_R.

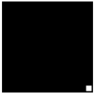
Uniform Lower Bound on S_R

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

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

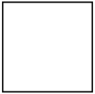
Slit Reference

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

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

Block Reference

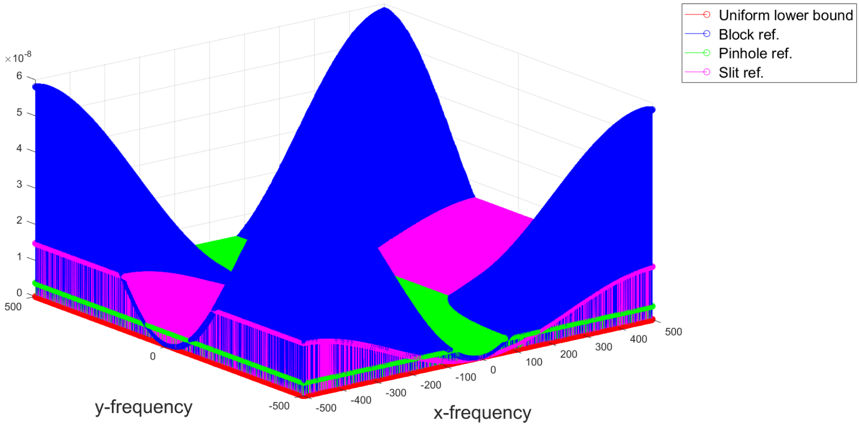
Theorem

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

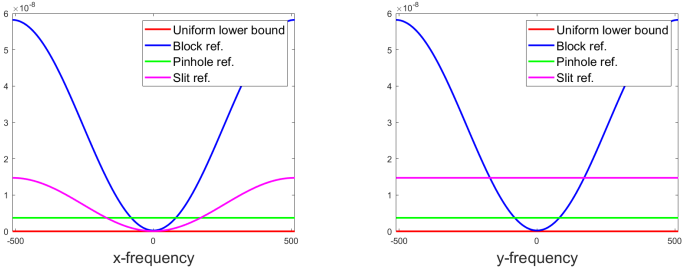
$$\frac{2n}{m^2} \max\left(1 - \cos(\frac{2\pi k_1}{m}), 1 - \cos(\frac{2\pi k_2}{m})\right). \tag{3.1}$$

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.

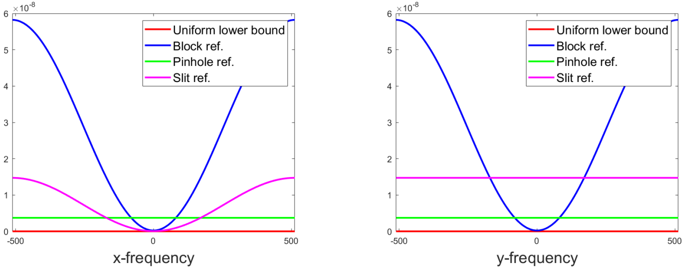
Frequency Scaling Comparison



Frequency Scaling Comparison (Border Cross-Sections)



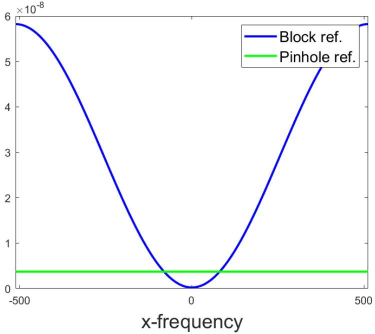
Frequency Scaling Comparison (Border Cross-Sections)



→ Tradeoffs between minimizing low or high frequencies

Can we get the best of both worlds?

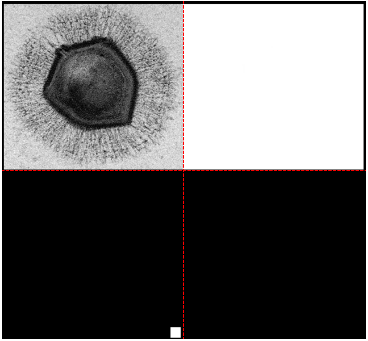
Block and Pinhole



Block → optimal for low-freq. scaling
Pinhole → optimal for high-freq. scaling

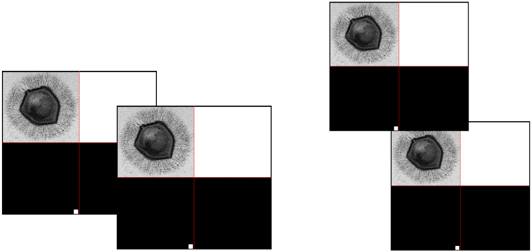
Dual-Reference

Let's try combining them!



$$\mathcal{X} = \begin{bmatrix} X & R_B \\ R_P & \mathbf{0}_{n\times n} \end{bmatrix}$$

Autocorrelation contains clean copies of specimen-block and specimen-pinhole cross-correlations



Recovery Algorithm

So two systems of equations:

$$M_{R_B}\,\mathrm{vec}(X) = \mathrm{vec}(C^{\diamond}_{[X,R_B]}),$$

and

$$M_{R_P}\,\mathrm{vec}(X) = \mathrm{vec}(C^{\diamond}_{[X,R_P]}).$$

Recovery Algorithm

Stack these two systems:

$$\begin{bmatrix} M_{R_B} \\ M_{R_P} \end{bmatrix} \mathrm{vec}(X) = \begin{bmatrix} \mathrm{vec}(C^{\diamond}_{[X,R_B]}) \\ \mathrm{vec}(C^{\diamond}_{[X,R_P]}) \end{bmatrix}.$$

Recovery Algorithm

Take the least-squares solution:

$$\min_{X \in \mathbb{C}^{n \times n}} \left\| M \operatorname{vec}(X) - b \right\|^2,$$

where $M = \begin{bmatrix} M_{R_B} \\ M_{R_P} \end{bmatrix}, b = \begin{bmatrix} \operatorname{vec}(C^{\diamond}_{[X,R_B]}) \\ \operatorname{vec}(C^{\diamond}_{[X,R_P]}) \end{bmatrix}$.

Recovery Algorithm

Take the least-squares solution:

$$\min_{X \in \mathbb{C}^{n \times n}} \left\| M \operatorname{vec}(X) - b \right\|^2,$$

where $M = \begin{bmatrix} M_{R_B} \\ M_{R_P} \end{bmatrix}, b = \begin{bmatrix} \operatorname{vec}(C^{\diamond}_{[X,R_B]}) \\ \operatorname{vec}(C^{\diamond}_{[X,R_P]}) \end{bmatrix}.$

Hence,

$$\operatorname{vec}(X) = M^{\dagger} b = (M^T M)^{-1} M^T b.$$

Recovery Algorithm

Definition

- Let $F \in \mathbb{C}^{m\times(4n-1)}$ be given by $F(k,t) = e^{-2\pi i k t/m}\ \forall\ (k,t) \in \{0,\ldots,m-1\}\times\{-(2n-1),\ldots,2n-1\}$.
- $Y = \mathcal{F}(\mathcal{X}) = F\mathcal{X}F^T$.
- Let $\mathcal{P}_{1B}, \mathcal{P}_{2B}, \mathcal{P}_{1P}, \mathcal{P}_{2P} \in \mathbb{R}^{n\times(4n-1)}$ be given by $\mathcal{P}_{1B} = \mathcal{P}_{2P} = [\mathbf{0}_{n\times n}, I_n, \mathbf{0}_{n\times(2n-1)}]$, and $\mathcal{P}_{2B} = \mathcal{P}_{1P} = [I_n, \mathbf{0}_{n\times(3n-1)}]$.
- Let $B_1 = \mathcal{P}_{2B}F^*, B_2 = \mathcal{P}_{1B}F^*, P_1 = \mathcal{P}_{2P}F^*, P_2 = \mathcal{P}_{1P}F^*$.

$$\mathrm{vec}(X) = T_{R_D}\,\mathrm{vec}(Y),$$

where

$$T_{R_D} = \frac{1}{m^2}M^\dagger\begin{bmatrix} B_1 \otimes B_2 \\ P_1 \otimes P_2 \end{bmatrix}.$$

Noisy Data

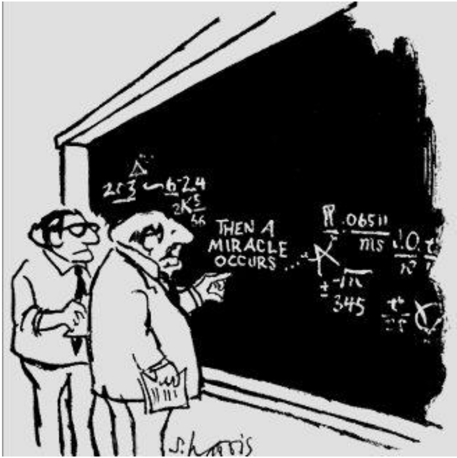
Given $Y^\star$, a possibly noise-corrupted version of $Y = |\mathcal{F}(\mathcal{X})|^2$, this procedure, – the **Referenced Deconvolution Algorithm** – gives $X^\star$, the solution of

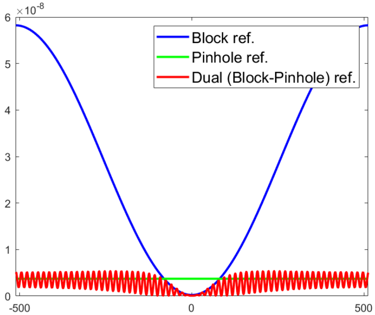
$$\min_X \frac{1}{2}\left\| Y^\star - \left|\mathcal{F}(\mathcal{X})\right|^2 \right\|^2.$$

Error Analysis

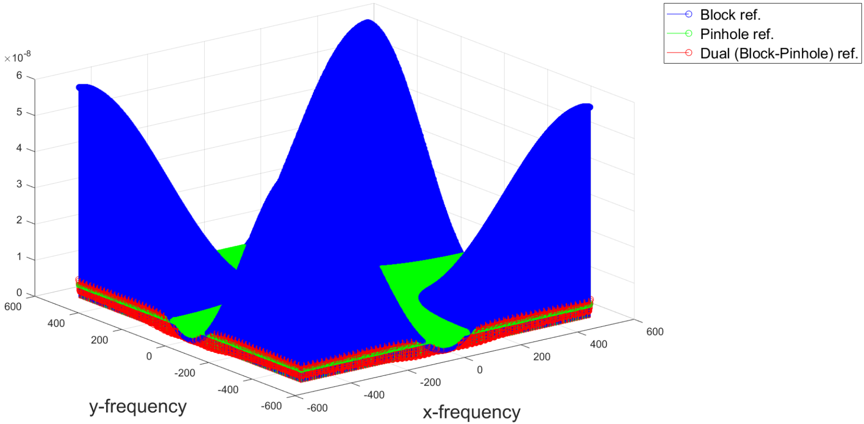
$$\mathbb{E}\|X^\star - X\|_F^2 = \left\langle S_{R_D}, \frac{\|Y\|_1}{N_p} Y \right\rangle_F,$$

where S_{R_D} is the dual-reference scaling factor.


THEN A
MIRACLE
OCCURS



→ Minimal scaling across the frequency spectrum!


Block ref.
Pinhole ref.
Dual (Block-Pinhole) ref.
×10^-8
6
5
4
3
2
1
0
600
400
200
0
-200
-400
-600
y-frequency
-600
-400
-200
0
200
400
600
x-frequency

Computing S_{R_D}

$$S_{R_D} = \mathsf{reshape}(\mathsf{diag}(T^*_{R_D} T_{R_D}), n, n).$$

Computing S_{R_D}

$$S_{R_D} = \mathsf{reshape}(\mathsf{diag}(T_{R_D}^* T_{R_D}), n, n).$$

Or,

$$S_{R_D}(k_1, k_2) = \|T_{R_D}(mk_1 + k_2, :)\|^2.$$

Computing S_{R_D}

$$S_{R_D} = \text{reshape}(\text{diag}(T^*_{R_D} T_{R_D}), n, n).$$

Or,

$$S_{R_D}(k_1, k_2) = \|T_{R_D}(mk_1 + k_2, :)\|^2.$$

$\rightarrow$ Can be highly parallelized, and leverage Kronecker factorization in T_{R_D}

Analytical Form of S_{R_D}

Definition

For $t, s \in \{0, \ldots, n-1\}$, let

$$u_s(t) = \frac{1}{\sqrt{\frac{n}{2} + \frac{1}{4}}} \sin \frac{(s + \frac{1}{2})(t+1)}{n + \frac{1}{2}} \pi,$$

$$v_s(t) = \frac{1}{\sqrt{\frac{n}{2} + \frac{1}{4}}} \cos \frac{(s + \frac{1}{2})(t+\frac{1}{2})}{n + \frac{1}{2}} \pi,$$

and

$$\sigma_s = [2 - 2\cos(\frac{s + \frac{1}{2}}{n + \frac{1}{2}} \pi)]^{-1/2}.$$

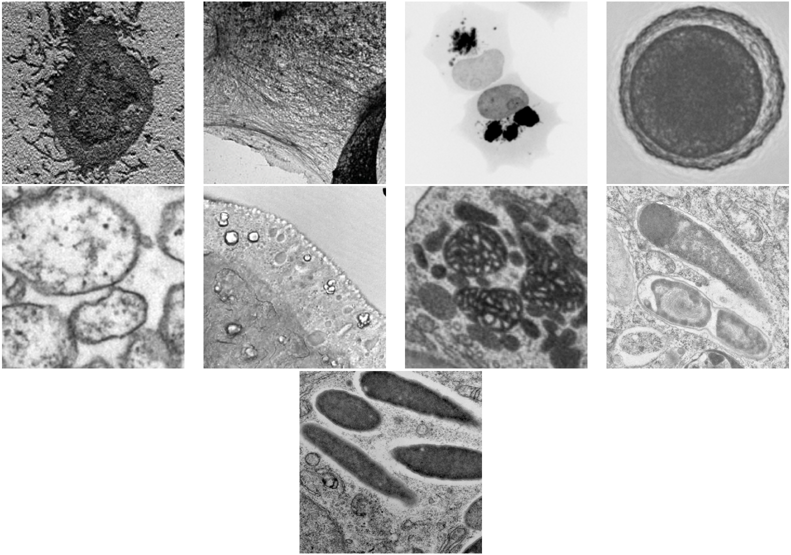
Analytical Form of S_{R_D}

Theorem

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

$$S_{R_D}(k_1, k2) = \frac{1}{m^4} \sum_{r,s=0}^{n-1} \left| \frac{\sigma_r \sigma_s}{\sigma_r^2 \sigma_s^2 + 1} u_r^\top B_1(:, k_1) u_s^\top B_2(:, k_2) + \frac{1}{\sigma_r^2 \sigma_s^2 + 1} v_r^\top P_1(:, k_1) v_s^\top P_2(:, k_2) \right|^2.$$

Test Images

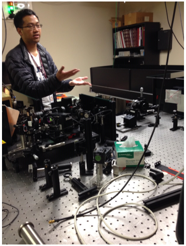


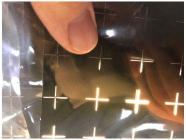
Recovery From Noisy Simulated Data

Image	Block Ref.	Pinhole Ref.	Dual Ref.	HIO
Mimivirus	3.70 (3.79)	46.9 (63.8)	1.51 (1.45)	93.7
Influenza	18.7 (18.5)	50.7 (31.4)	4.64 (4.70)	695
Stroma cells	9.19 (8.91)	23.1 (44.1)	2.78 (2.63)	1607
mCherry proteins	1.84 (1.84)	139 (131)	0.927 (0.908)	403
Embryo	6.30 (6.29)	54.2 (53.8)	2.62 (2.71)	642
Oocytes	7.01 (6.83)	44.1 (78.3)	2.66 (2.70)	883
S. pistallata	4.02 (3.93)	148 (83.7)	1.29 (1.31)	335
Aragonite	11.6 (11.5)	52.1 (34.6)	4.41 (4.41)	1767
Salmonella WT	9.07 (8.81)	44.3 (60.1)	3.33 (2.97)	708
sifA	7.27 (7.15)	42.6 (54.6)	2.82 (2.86)	1765

Table: Empirical (and expected) relative errors, scaled by 10^{-4}

SLAC Experiment





Thank you!