Thesis Defense

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Thesis Overview

The Phase Retrieval Problem

$$\textbf{Given} \quad Y_{\mathbf{k}} = |\mathcal{A}(X)_{\mathbf{k}}|^2, \quad \mathbf{k} \in \mathcal{K}$$
$$\textbf{Recover} \quad X,$$

where $\mathcal{A}$ is a known linear operator.

Fourier Phase Retrieval

Given $Y_{\mathbf{k}} = |\mathcal{A}(X)_{\mathbf{k}}|^2, \quad \mathbf{k} \in \mathcal{K}$

Recover X.

- Fourier phase retrieval: $Y = |\mathcal{F}(X)|^2$, where $\mathcal{F}$ is a Fourier transform operator.
- Occurs in scientific imaging — diffraction imaging, optics, crystallography.

Gaussian Phase Retrieval

Given $Y_{\mathbf{k}} = |\mathcal{A}(X)_{\mathbf{k}}|^2, \quad \mathbf{k} \in \mathcal{K}$
Recover $X.$

- Gaussian phase retrieval: $y_k = |\mathbf{a}_k^T \mathbf{x}|, k = 1, \ldots, m$, where $\mathbf{a}_k$'s are Gaussian vectors.
- System of random quadratic equations.

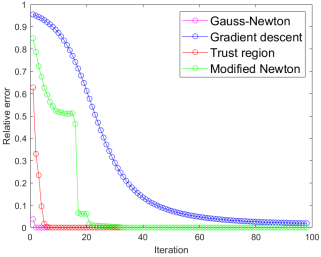
Holographic Phase Retrieval and Reference Design

Introduces a general mathematical and statistical framework for the *holographic phase retrieval* problem, and proposes a new *dual-reference* design.

- *On Block-Reference Coherent Diffraction Imaging*
  David A. Barmherzig, Ju Sun, T.J. Lane, and Po-Nan Li. *OSA Imaging and Applied Optics Congresss*, 2018.
- *Holographic Phase Retrieval and Optimal Reference Design*
  David A. Barmherzig, Ju Sun, Po-Nan Li, T.J. Lane, and Emmanuel J. Candès. *Inverse Problems*, 2019.
- *Dual-Reference Design for Holographic Coherent Diffraction Imaging*
  David A. Barmherzig, Ju Sun, Po-Nan Li, T.J. Lane, and Emmanuel J. Candès. *SampTA*, 2019.

Theory and Algorithms for 1D Fourier Phase Retrieval

- Problem theory
- Semidefinite programming recovery methods
- Least-squares recovery methods



1D Phase Retrieval and Spectral Factorization
David Barmherzig and Ju Sun. *OSA Congress on Imaging and Applied Optics*, 2018.

Biconvex Optimization for Gaussian Phase Retrieval

- Formulate Gaussian phase retrieval ($y_k = |\mathbf{a}_k^T \mathbf{x}|, k = 1, \cdots, m$) as a *biconvex* and *biquadratic* optimization problem:

$$\begin{aligned} \text{minimize}_{\mathbf{z},\mathbf{w}\in\mathbb{R}^n} \quad & f(\mathbf{z},\mathbf{w}) \doteq \frac{1}{4m}\sum_{k=1}^{m}(y_k - \mathbf{a}_k^T\mathbf{z}\mathbf{a}_k^T\mathbf{w})^2 \\ \text{subject to} \quad & \mathbf{z} = \mathbf{w}. \end{aligned}$$

- Optimization via ADMM and block coordinate descent
- Proof of linear convergence using block coordinate descent

A Local Analysis of Block Coordinate Descent for Gaussian Phase Retrieval David Barmherzig and Ju Sun. 10^{th} NIPS Workshop on Optimization for Machine Learning, 2017.

Holographic Phase Retrieval and Reference Design

Coherent Diffraction Imaging (CDI)

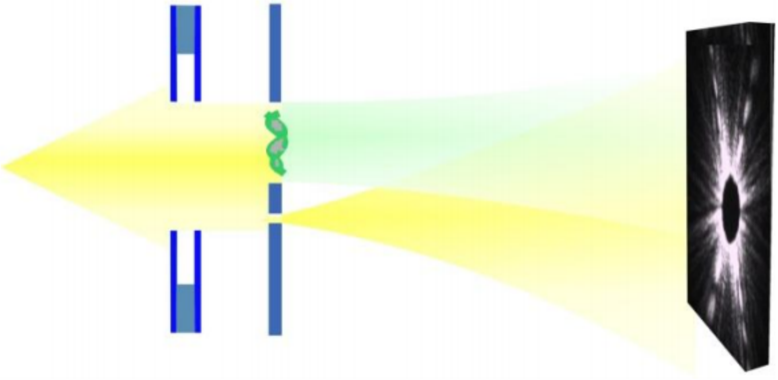
The Phase Retrieval Problem in CDI

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

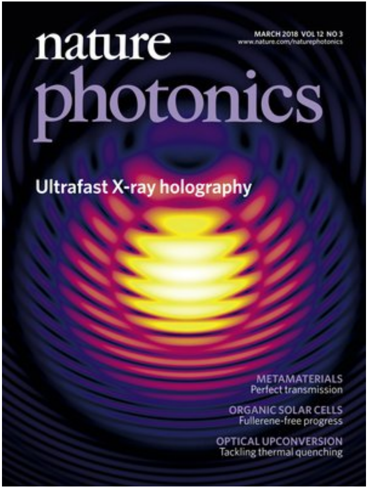
Can *discretize* this problem as:

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

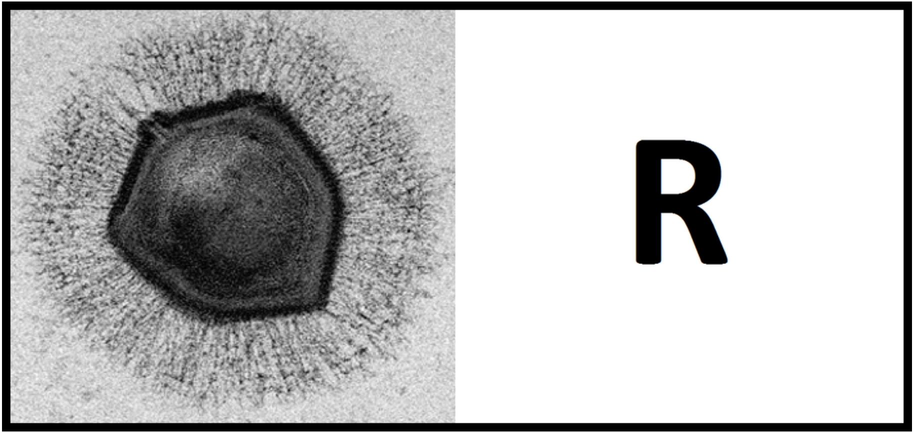
Holographic CDI



Holographic CDI



Specimen and Reference Setup



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!

We will now achieve:

- Uniqueness guarantee
- Algorithm with provable recovery
- Closed-form expression — a linear operation! — rather than iterative

Algorithm: *Referenced Deconvolution*

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

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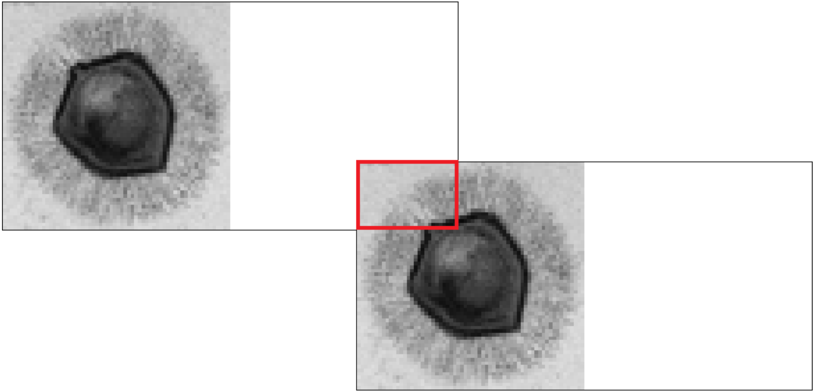
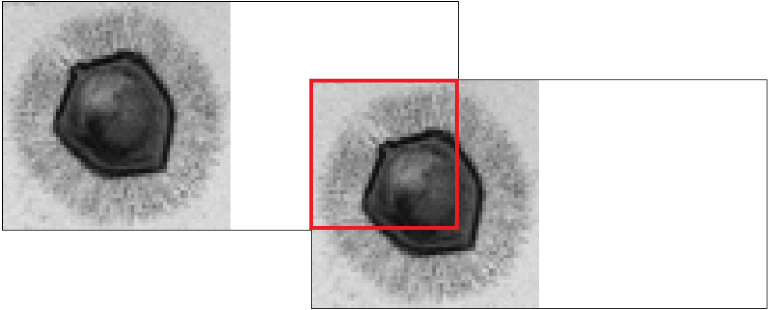
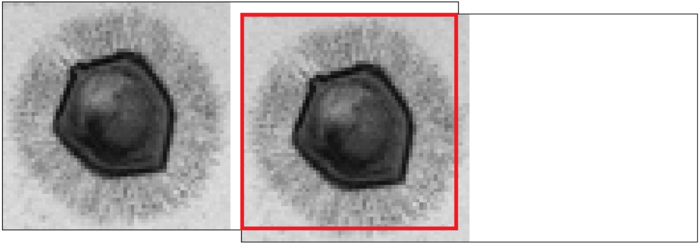
Step 2: Extract $C^{\diamond}_{[X,R]}$, the top-left quadrant of $A_{[X,R]}$. *This is one quadrant of the cross-correlation of X and R.*







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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: Deconvolve X and R.

$$\operatorname{vec}(X) = M_R^{-1} \operatorname{vec}(C^{\diamond}_{[X,R]}).$$

For

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

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

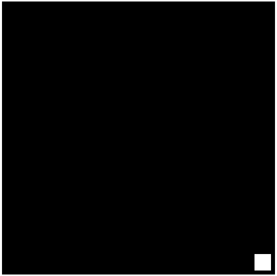
Altogether, this gives a linear relationship between $Y = \left|\widehat{[X, R]}\right|^2$ and X!

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

Special Cases

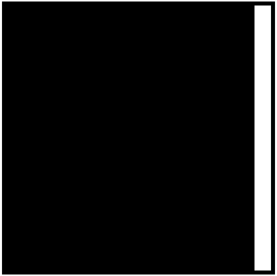
For popular reference choices, M_R has a special structure.

Pinhole Reference



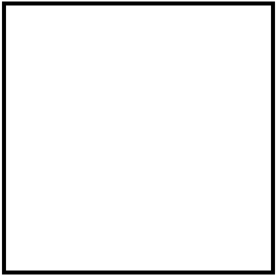
$M_R = I_{n^2}$.

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 Analysis

Error Formula

Recovery from clean and noisy data, respectively:

- $\mathrm{vec}(X) = T_R \,\mathrm{vec}(Y)$
- $\mathrm{vec}(\widetilde{X}) = T_R \,\mathrm{vec}(\widetilde{Y})$

Expected recovery error:

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

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

$$\widetilde{Y} \sim_{\text{ind}} \frac{\|Y\|_1}{N_p}\mathrm{Pois}\Big(\frac{N_p}{\|Y\|_1}Y\Big).$$

Poisson noise error formula

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

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

Poisson noise error formula

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

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.

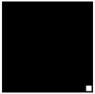
Uniform Lower Bound on S_R

Theorem

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

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

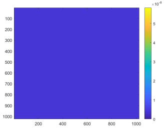
Pinhole Reference



Theorem

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

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

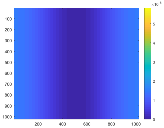


Slit Reference

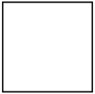
Theorem

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

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



Block Reference

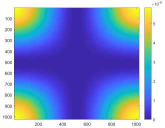


Theorem

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

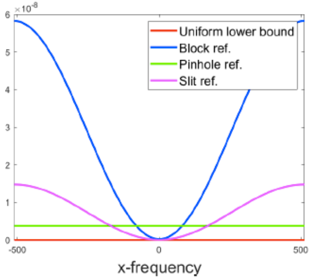
Theorem

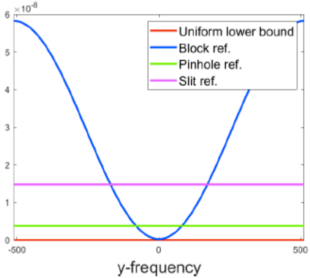
For the block reference R_b, $S_{R_b}(k_1, k_2)$ deviates from the uniform lower bound on $S_R(k_1, k_2)$ at a rate of

$$\frac{2n}{m^2} \max\left(1 - \cos(\frac{2\pi k_1}{m}), 1 - \cos(\frac{2\pi k_2}{m})\right). \quad (4.1)$$

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 (Border Cross-Sections)





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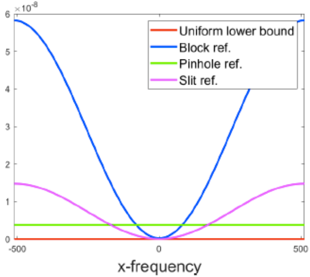
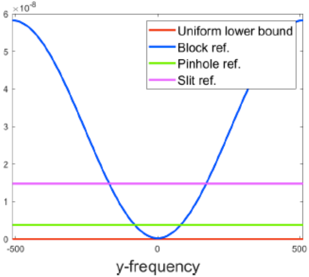
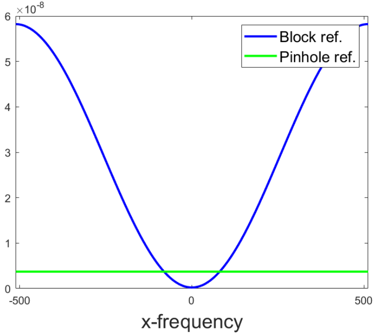




$\rightarrow$ Tradeoffs between minimizing low or high frequencies

Can we get the best of both worlds?

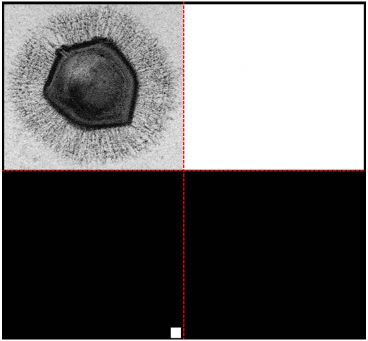
Recall:



Block → good (optimal) for low-frequency scaling
Pinhole → good for high-frequency scaling

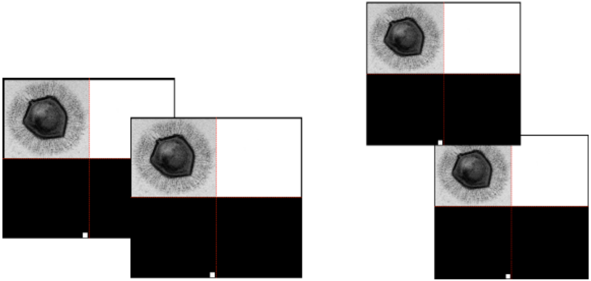
Dual-Reference

Let's try combining them!



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

Careful placement ensures the autocorrelation contains *non-overlapping copies* of the 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:

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

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:

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

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

Hence,

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

Recovery Algorithm

Gives linear recovery of signal X from data Y:

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

where

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

and

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

Error Analysis

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

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

Analytical Form of S_{R_D}

Definition

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

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

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

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

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

Computing S_{R_D}

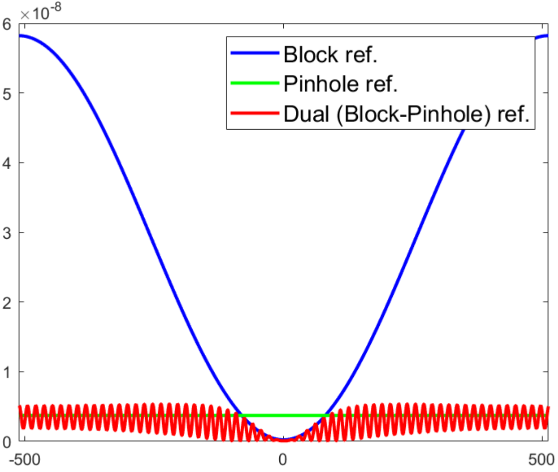
$$S_{R_D} = \text{reshape}(\text{diag}(T_{R_D}^* T_{R_D}), n, n).$$

Or,

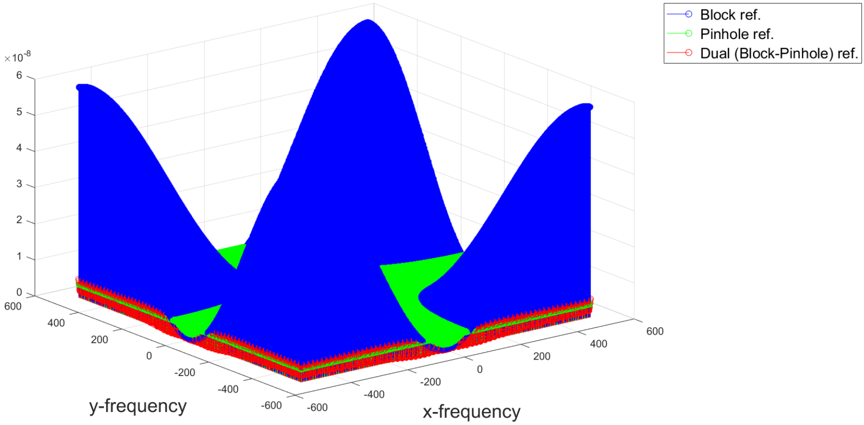
$$S_{R_D}(k_1, k_2) = \|T_{R_D}(mk_1 + k_2, :)\|^2.$$

$\rightarrow$ Can leverage Kronecker product factorization of T_{R_D} to make this highly parallelized

The moment of truth...

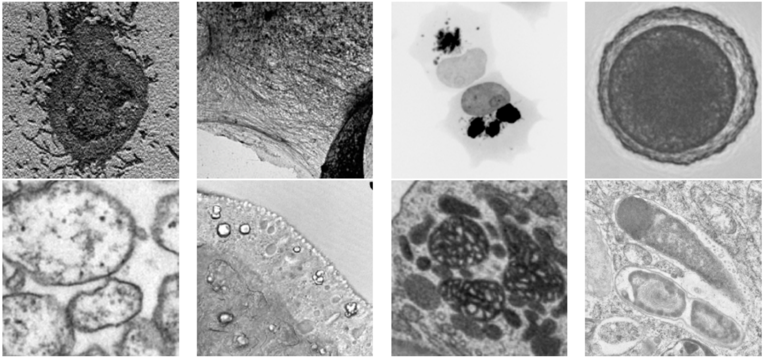


→ Minimal error scaling across the frequency spectrum!



×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
Block ref.
Pinhole ref.
Dual (Block-Pinhole) ref.

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}.

The Future

Optical/CDI experiments in development...!

Thank you!

- Professor Emmanuel Candès
- Professor Walter Murray
- Professor Gordon Wetzstein
- Professor Jon Claerbout
- Professor Peter Kitanidis
- Dr. Ju Sun
- Dr. T.J. Lane and Po-Nan Li
- And many other collaborators, colleagues, and friends!