

Stability Estimates for Linearized Near-Field Phase Retrieval in X-Ray Phase Contrast Imaging

A Well-posed Phase Retrieval Problem

Simon Maretzke, Thorsten Hohage

SFB 755 - Nanoscale Photonic Imaging

Oberwolfach Workshop "Computational Inverse Problems for Partial Differential
Equations"

May 16, 2017

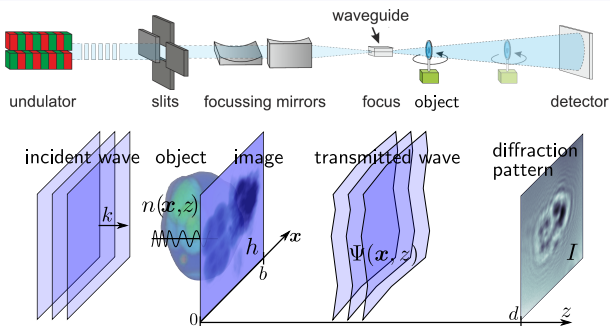


GEORG-AUGUST-UNIVERSITÄT
GÖTTINGEN



Introduction

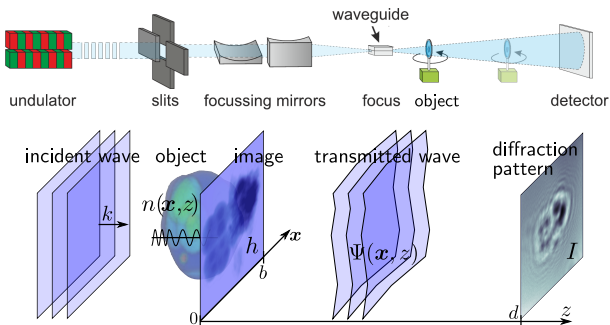
Experimental Setup: X-Ray Phase Contrast Imaging¹



- Sample (e.g. biological cell) illuminated by coherent X-rays
 ↳ plane electromagnetic wave, *single* wavenumber $k \gg 1$

¹Salditt, T et Al. (2015). *Journal of Synchrotron Radiation* **22**(4): 867-878.

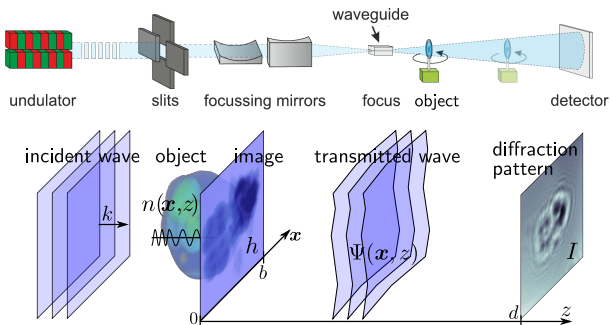
Experimental Setup: X-Ray Phase Contrast Imaging¹



- Sample (e.g. biological cell) illuminated by coherent X-rays
 \rightsquigarrow plane electromagnetic wave, *single* wavenumber $k \gg 1$
- *Intensity* of diffracted wavefield (*hologram*) measured at finite distance $d > 0$ behind the object (\rightsquigarrow *phase problem*)

¹ Salditt, T et Al. (2015). *Journal of Synchrotron Radiation* **22**(4): 867-878.

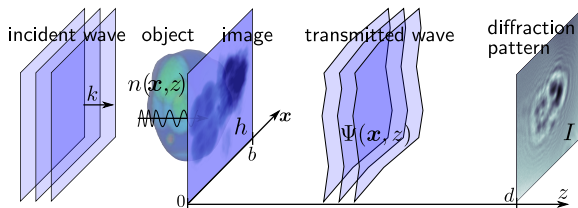
Experimental Setup: X-Ray Phase Contrast Imaging¹



- Sample (e.g. biological cell) illuminated by coherent X-rays
 \rightsquigarrow plane electromagnetic wave, *single* wavenumber $k \gg 1$
- *Intensity* of diffracted wavefield (*hologram*) measured at finite distance $d > 0$ behind the object (\rightsquigarrow *phase problem*)
- *Inverse problem:* Recover the image h (= wavefield perturbation)

¹Salditt, T et Al. (2015). *Journal of Synchrotron Radiation* **22**(4): 867-878.

Imaging Model



Parameters:

$$n = 1 - \delta + i\beta$$

refractive index

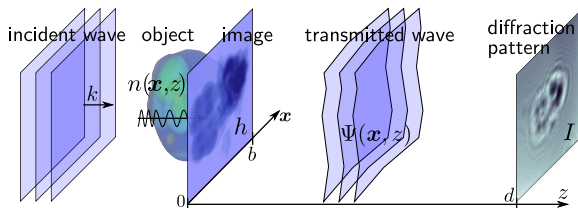
$$N_F = kb^2/d \sim 10^{2...4}$$

Fresnel number

$$\text{Forward Model: } F : h = ik \int (n-1) dz \mapsto I = \left| \underbrace{\mathcal{D}}_{\text{Fresnel propagator}} \underbrace{(\exp(h))}_{\text{exit wave field } \Psi(\mathbf{x}, 0)} \right|^2$$

Phase shifts
(+absorption)

Imaging Model



Parameters:

$$n = 1 - \delta + i\beta$$

refractive index

$$N_F = kb^2/d \sim 10^{2\dots 4}$$

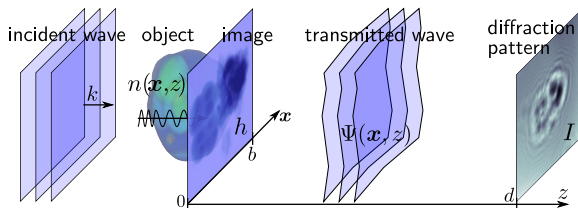
Fresnel number

$$\text{Forward Model: } F : h = ik \int (n - 1) dz \mapsto I = \left| \underbrace{\mathcal{D}}_{\text{Fresnel propagator}} \underbrace{(\exp(h))}_{\text{exit wave field } \Psi(\mathbf{x}, 0)} \right|^2$$

Phase shifts
(+absorption)

- *Basic Model:* Helmholtz equation $\Delta\Psi + n^2 k^2 \Psi = 0$

Imaging Model



Parameters:

$$n = 1 - \delta + i\beta$$

refractive index

$$N_F = kb^2/d \sim 10^{2...4}$$

Fresnel number

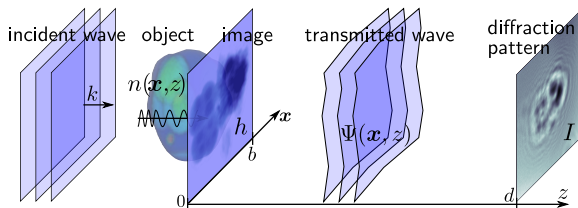
$$\text{Forward Model: } F : h = ik \int (n - 1) dz \mapsto I = \left| \underbrace{\mathcal{D}}_{\text{Fresnel propagator}} \underbrace{(\exp(h))}_{\text{exit wave field } \Psi(x,0)} \right|^2$$

Phase shifts
(+absorption)

- ▶ **Basic Model:** Helmholtz equation $\Delta\Psi + n^2 k^2 \Psi = 0$
- ▶ **Simplifications:** (\rightsquigarrow valid hard X-ray regime¹: thin objects, large k)
 - 1 Ray-optics description of wave-object interaction
 - 2 Paraxial approximation: $\Psi(x, z) = \exp(ikz)\tilde{\Psi}(x, z)$, $|\nabla\tilde{\Psi}| \ll k|\tilde{\Psi}|$

¹ Jonas, P and Louis, AK (2004). *Inverse Problems* **20**(1): 75.

Imaging Model



Parameters:

$$n = 1 - \delta + i\beta$$

refractive index

$$N_F = kb^2/d \sim 10^{2...4}$$

Fresnel number

$$\text{Forward Model: } F : h = ik \int (n - 1) dz \mapsto I = \left| \underbrace{\mathcal{D}}_{\substack{\text{Fresnel} \\ \text{propagator}}} \underbrace{(\exp(h))}_{\substack{\text{exit wave field} \\ \Psi(\mathbf{x}, 0)}} \right|^2$$

Phase shifts
(+absorption)

- ▶ **Basic Model:** Helmholtz equation $\Delta\Psi + n^2 k^2 \Psi = 0$
- ▶ **Simplifications:** (\rightsquigarrow valid hard X-ray regime¹: thin objects, large k)
 - 1 Ray-optics description of wave-object interaction
 - 2 Paraxial approximation: $\Psi(x, z) = \exp(ikz)\tilde{\Psi}(x, z)$, $|\nabla\tilde{\Psi}| \ll k|\tilde{\Psi}|$
- **Fresnel propagator:**

$$\mathcal{D} : \tilde{\Psi}(x, 0) \mapsto \tilde{\Psi}(x, d); \mathcal{D}(f) := \mathcal{F}^{-1} \left(\exp(-i\xi^2/(2N_F)) \cdot \mathcal{F}(f)(\xi) \right)$$

¹ Jonas, P and Louis, AK (2004). *Inverse Problems* **20**(1): 75.

Inverse Problem and Stability

Nonlinear forward model:

$$I = F(h) = |\mathcal{D}(\exp(h))|^2$$

Inverse Problem 1 (Phase retrieval in propagation imaging)

Recover an image $h \in A$ from observed intensity data $F(h) + \varepsilon$.

Inverse Problem and Stability

Linearized forward model: valid for “weak” perturbations h

$$I = F(h) = |\mathcal{D}(\exp(h))|^2 = 1 + Th + \cancel{O(h^2)} \quad \text{with} \quad Th := 2 \operatorname{Re}(\mathcal{D}(h)).$$

Inverse Problem 2 (Linearized phase retrieval in phase contrast imaging)

Recover an image $h \in A \subset L^2(\mathbb{R}^m)$ from observed intensities $1 + Th + \varepsilon$.

Inverse Problem and Stability

Linearized forward model: valid for “weak” perturbations h

$$I = F(h) = |\mathcal{D}(\exp(h))|^2 = 1 + Th + \cancel{O(h^2)} \quad \text{with} \quad Th := 2 \operatorname{Re}(\mathcal{D}(h)).$$

Inverse Problem 2 (Linearized phase retrieval in phase contrast imaging)

Recover an image $h \in A \subset L^2(\mathbb{R}^m)$ from observed intensities $1 + Th + \varepsilon$.

Uniqueness and stability:

- *Generally non-unique:* $\operatorname{kern}(T) = \{\mathcal{D}^{-1}(g) : g \in L^2(\mathbb{R}^m, i\mathbb{R})\}$

Inverse Problem and Stability

Linearized forward model: valid for “weak” perturbations h

$$I = F(h) = |\mathcal{D}(\exp(h))|^2 = 1 + Th + \cancel{O(h^2)} \quad \text{with} \quad Th := 2 \operatorname{Re}(\mathcal{D}(h)).$$

Inverse Problem 2 (Linearized phase retrieval in phase contrast imaging)

Recover an image $h \in A \subset L^2(\mathbb{R}^m)$ from observed intensities $1 + Th + \varepsilon$.

Uniqueness and stability:

- *Generally non-unique:* $\operatorname{kern}(T) = \{\mathcal{D}^{-1}(g) : g \in L^2(\mathbb{R}^m, i\mathbb{R})\}$
- *Paradigm:* Need in general two holograms I_1, I_2 with $N_{F,1} \neq N_{F,2}$ ²

²Jonas, P and Louis, AK (2004). *Inverse Problems* **20**(1): 75.

Inverse Problem and Stability

Linearized forward model: valid for “weak” perturbations h

$$I = F(h) = |\mathcal{D}(\exp(h))|^2 = 1 + Th + \cancel{O(h^2)} \quad \text{with} \quad Th := 2 \operatorname{Re}(\mathcal{D}(h)).$$

Inverse Problem 2 (Linearized phase retrieval in phase contrast imaging)

Recover an image $h \in A \subset L^2(\mathbb{R}^m)$ from observed intensities $1 + Th + \varepsilon$.

Uniqueness and stability:

- *Generally non-unique:* $\operatorname{kern}(T) = \{\mathcal{D}^{-1}(g) : g \in L^2(\mathbb{R}^m, i\mathbb{R})\}$
- *Paradigm:* Need in general two holograms I_1, I_2 with $N_{F,1} \neq N_{F,2}^2$
- ✓ *Uniqueness result*³: IP2 (and IP1 up to phase-periodicity) uniquely solvable for *compactly supported* h

²Jonas, P and Louis, AK (2004). *Inverse Problems* **20**(1): 75.

³SCM (2015). *Inverse Problems* **31**: 065003.

Inverse Problem and Stability

Linearized forward model: valid for “weak” perturbations h

$$I = F(h) = |\mathcal{D}(\exp(h))|^2 = 1 + Th + \cancel{O(h^2)} \quad \text{with} \quad Th := 2 \operatorname{Re}(\mathcal{D}(h)).$$

Inverse Problem 2 (Linearized phase retrieval in phase contrast imaging)

Recover an image $h \in A \subset L^2(\mathbb{R}^m)$ from observed intensities $1 + Th + \varepsilon$.

Uniqueness and stability:

- *Generally non-unique:* $\operatorname{kern}(T) = \{\mathcal{D}^{-1}(g) : g \in L^2(\mathbb{R}^m, i\mathbb{R})\}$
- *Paradigm:* Need in general two holograms I_1, I_2 with $N_{F,1} \neq N_{F,2}^2$
- ✓ *Uniqueness result*³: IP2 (and IP1 up to phase-periodicity) uniquely solvable for *compactly supported* h
- ? *Analyze stability* to noise ε to see what can be recovered in practice
 ↪ *This talk!*

²Jonas, P and Louis, AK (2004). *Inverse Problems* **20**(1): 75.

³SCM (2015). *Inverse Problems* **31**: 065003.

Stability Analysis of the Linearized Problem

Preliminaries

Facts about the Fresnel propagator:

- 1 $\mathcal{D} : L^2(\mathbb{R}^m) \rightarrow L^2(\mathbb{R}^m)$ is unitary: $\mathcal{F} \mathcal{D}(h) = \underbrace{\exp(-i\xi^2/(2N_F))}_{\text{unitary}} \cdot \mathcal{F}(h)$
- 2 Inversion by complex conjugation: $\overline{\mathcal{D}(h)} = \mathcal{D}^{-1}(\bar{h})$

- 3 Alternate form: \mathcal{D} can be rewritten via the convolution theorem

$$\mathcal{D}(h) = e^{-im\pi/4} N_F^{\frac{m}{2}} n_F \cdot \mathcal{F}(n_F \cdot h)(N_F \cdot), \quad n_F(\mathbf{x}) := \exp\left(\frac{iN_F \mathbf{x}^2}{2}\right)$$

Preliminaries

Facts about the Fresnel propagator:

1 $\mathcal{D} : L^2(\mathbb{R}^m) \rightarrow L^2(\mathbb{R}^m)$ is unitary: $\mathcal{F} \mathcal{D}(h) = \underbrace{\exp(-i\xi^2/(2N_F))}_{\text{unitary}} \cdot \mathcal{F}(h)$

2 Inversion by complex conjugation: $\overline{\mathcal{D}(h)} = \mathcal{D}^{-1}(\bar{h})$

3 Alternate form: \mathcal{D} can be rewritten via the convolution theorem

$$\mathcal{D}(h) = e^{-im\pi/4} N_F^{\frac{m}{2}} n_F \cdot \mathcal{F}(n_F \cdot h)(N_F \cdot), \quad n_F(\mathbf{x}) := \exp\left(\frac{iN_F \mathbf{x}^2}{2}\right)$$

Twin-image problem: Alternative interpretation of T via 2

$$Th = 2 \operatorname{Re}(\mathcal{D}(h)) = \mathcal{D}(h) + \overline{\mathcal{D}(h)} = \underbrace{\mathcal{D}(h)}_{\text{propagated image}} + \underbrace{\mathcal{D}^{-1}(\bar{h})}_{\text{back-propagated twin-image}}$$

Preliminaries

Facts about the Fresnel propagator:

1 $\mathcal{D} : L^2(\mathbb{R}^m) \rightarrow L^2(\mathbb{R}^m)$ is unitary: $\mathcal{F} \mathcal{D}(h) = \underbrace{\exp(-i\xi^2/(2N_F))}_{\text{unitary}} \cdot \mathcal{F}(h)$

2 Inversion by complex conjugation: $\overline{\mathcal{D}(h)} = \mathcal{D}^{-1}(\bar{h})$

3 Alternate form: \mathcal{D} can be rewritten via the convolution theorem

$$\mathcal{D}(h) = e^{-im\pi/4} N_F^{\frac{m}{2}} n_F \cdot \mathcal{F}(n_F \cdot h)(N_F \cdot), \quad n_F(\mathbf{x}) := \exp\left(\frac{iN_F \mathbf{x}^2}{2}\right)$$

Twin-image problem: Alternative interpretation of T via 2

$$Th = 2 \operatorname{Re}(\mathcal{D}(h)) = \mathcal{D}(h) + \overline{\mathcal{D}(h)} = \underbrace{\mathcal{D}(h)}_{\text{propagated image}} + \underbrace{\mathcal{D}^{-1}(\bar{h})}_{\text{back-propagated twin-image}}$$

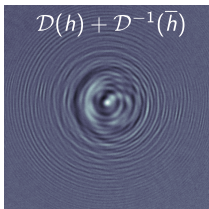
- ▶ \mathcal{D} unitary \Rightarrow Stable inversion iff summands can be distinguished
- ▶ How to disentangle image- and twin-image contributions?

Resolving the Twin-image Problem

Gabor Holography²:

Propagate data such that twin-image is *in-focus*:

$$\mathcal{D}(Th) = \mathcal{D}(\mathcal{D}(h) + \mathcal{D}^{-1}(\bar{h})) = \mathcal{D}^2(h) + \bar{h}$$



²Gabor, D et Al. (1948). *Nature* **161**(4098): 777-778. (Nobel Prize in Physics 1971)

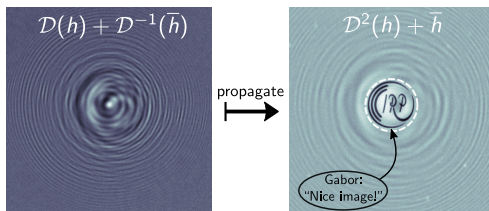
Resolving the Twin-image Problem

Gabor Holography²:

Propagate data such that twin-image is *in-focus*:

$$\mathcal{D}(Th) = \mathcal{D}(\mathcal{D}(h) + \mathcal{D}^{-1}(\bar{h})) = \mathcal{D}^2(h) + \bar{h}$$

- ▶ Yields sharp twin-image \bar{h} perturbed by twice propagated image
 \rightsquigarrow *qualitative* image recovery



²Gabor, D et Al. (1948). *Nature* **161**(4098): 777-778. (Nobel Prize in Physics 1971)

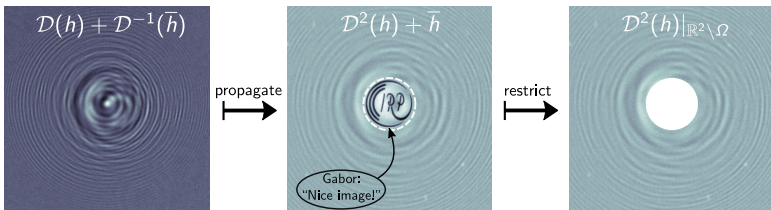
Resolving the Twin-image Problem

Gabor Holography²:

Propagate data such that twin-image is *in-focus*:

$$\mathcal{D}(Th) = \mathcal{D}(\mathcal{D}(h) + \mathcal{D}^{-1}(\bar{h})) = \mathcal{D}^2(h) + \bar{h}$$

- ▶ Yields sharp twin-image \bar{h} perturbed by twice propagated image
 \rightsquigarrow *qualitative* image recovery
- ▶ $\mathcal{D}^2(h)|_{\mathbb{R}^m \setminus \Omega}$ can be identified by *restriction* if $\text{supp}(h) \subset \Omega$



²Gabor, D et Al. (1948). *Nature* **161**(4098): 777-778. (Nobel Prize in Physics 1971)

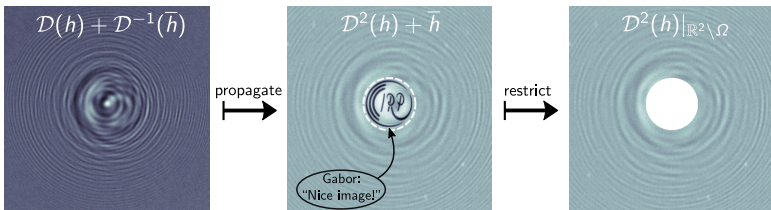
Resolving the Twin-image Problem

Gabor Holography²:

Propagate data such that twin-image is *in-focus*:

$$\mathcal{D}(Th) = \mathcal{D}(\mathcal{D}(h) + \mathcal{D}^{-1}(\bar{h})) = \mathcal{D}^2(h) + \bar{h}$$

- ▶ Yields sharp twin-image \bar{h} perturbed by twice propagated image
 \rightsquigarrow qualitative image recovery
- ▶ $\mathcal{D}^2(h)|_{\mathbb{R}^m \setminus \Omega}$ can be identified by *restriction* if $\text{supp}(h) \subset \Omega$



\rightsquigarrow Elimination of twin-image at the expense of data incompleteness

²Gabor, D et Al. (1948). *Nature* **161**(4098): 777-778. (Nobel Prize in Physics 1971)

Reduction to Fourier Completion Problem

Theorem 3 (Stability in terms of Fourier completion problem)

Let T denote the forward operator of IP2 and let $\text{supp}(h) \subset \Omega$ for some measurable set $\Omega \subset \mathbb{R}^m$. Define $\Omega_F := \{(N_F/2)\mathbf{x} : \mathbf{x} \in \Omega\}$. Then

$$\|Th\| \geq \|\mathcal{F}(n_F^{1/2} \cdot h)|_{\Omega_F^c}\|.$$

In particular, we have the stability estimate

$$\|Th\| \geq C_{\text{IP2}} \|h\| \quad \text{with} \quad C_{\text{IP2}} := \inf_{h \in L^2(\Omega), \|h\|=1} \|\mathcal{F}(h)|_{\Omega_F^c}\|$$

Reduction to Fourier Completion Problem

Theorem 3 (Stability in terms of Fourier completion problem)

Let T denote the forward operator of IP2 and let $\text{supp}(h) \subset \Omega$ for some measurable set $\Omega \subset \mathbb{R}^m$. Define $\Omega_F := \{(N_F/2)\mathbf{x} : \mathbf{x} \in \Omega\}$. Then

$$\|Th\| \geq \|\mathcal{F}(n_F^{1/2} \cdot h)|_{\Omega_F^c}\|.$$

In particular, we have the stability estimate

$$\|Th\| \geq C_{\text{IP2}} \|h\| \quad \text{with} \quad C_{\text{IP2}} := \inf_{h \in L^2(\Omega), \|h\|=1} \|\mathcal{F}(h)|_{\Omega_F^c}\|$$

Proof:

- ▶ Holographic approach: $\|Th\| = \|\mathcal{D}Th\| \geq \|\mathcal{D}Th|_{\Omega^c}\| = \|\mathcal{D}^2(h)|_{\Omega^c}\|$

Reduction to Fourier Completion Problem

Theorem 3 (Stability in terms of Fourier completion problem)

Let T denote the forward operator of IP2 and let $\text{supp}(h) \subset \Omega$ for some measurable set $\Omega \subset \mathbb{R}^m$. Define $\Omega_F := \{(N_F/2)\mathbf{x} : \mathbf{x} \in \Omega\}$. Then

$$\|Th\| \geq \|\mathcal{F}(n_F^{1/2} \cdot h)|_{\Omega_F^c}\|.$$

In particular, we have the stability estimate

$$\|Th\| \geq C_{\text{IP2}} \|h\| \quad \text{with} \quad C_{\text{IP2}} := \inf_{h \in L^2(\Omega), \|h\|=1} \|\mathcal{F}(h)|_{\Omega_F^c}\|$$

Proof:

- ▶ Holographic approach: $\|Th\| = \|\mathcal{D}Th\| \geq \|\mathcal{D}Th|_{\Omega^c}\| = \|\mathcal{D}^2(h)|_{\Omega^c}\|$
- ▶ Alternate form: $\mathcal{D}^2(h) = \underbrace{e^{-im\pi/4} n_F^{1/2}}_{\text{unitary}} \cdot (N_F/2)^{\frac{m}{2}} \mathcal{F}(n_F^{1/2} \cdot h) \cdot ((N_F/2) \cdot \cdot)$

Reduction to Fourier Completion Problem

Theorem 3 (Stability in terms of Fourier completion problem)

Let T denote the forward operator of IP2 and let $\text{supp}(h) \subset \Omega$ for some measurable set $\Omega \subset \mathbb{R}^m$. Define $\Omega_F := \{(N_F/2)\mathbf{x} : \mathbf{x} \in \Omega\}$. Then

$$\|Th\| \geq \|\mathcal{F}(n_F^{1/2} \cdot h)|_{\Omega_F^c}\|.$$

In particular, we have the stability estimate

$$\|Th\| \geq C_{\text{IP2}} \|h\| \quad \text{with} \quad C_{\text{IP2}} := \inf_{h \in L^2(\Omega), \|h\|=1} \|\mathcal{F}(h)|_{\Omega_F^c}\|$$

Proof:

- ▶ Holographic approach: $\|Th\| = \|\mathcal{D}Th\| \geq \|\mathcal{D}Th|_{\Omega^c}\| = \|\mathcal{D}^2(h)|_{\Omega^c}\|$
- ▶ Alternate form: $\mathcal{D}^2(h) = \underbrace{e^{-im\pi/4} n_F^{1/2}}_{\text{unitary}} \cdot (N_F/2)^{\frac{m}{2}} \mathcal{F}(n_F^{1/2} \cdot h)((N_F/2) \cdot \cdot)$
- ▶ Insert and rescale □

Well-Posedness and Stability Result

Theorem 4 (Well-posedness and stability estimate for $IP2^4$)

Let $A := \{h \in L^2(\mathbb{R}^m) : \text{supp}(h) \subset \Omega\}$ with supporting domain Ω given by a stripe of width 1, w.l.o.g. $\Omega := [-\frac{1}{2}; \frac{1}{2}] \times \mathbb{R}^{m-1}$. Then

$$\|Th\| \geq C_{IP2}(\Omega, N_F) \|h\| \quad \text{for all } h \in A,$$

where the stability constant $C_{IP2}(\Omega, N_F) > 0$ satisfies the estimate

$$C_{IP2}(\Omega, N_F) \geq (2\pi N_F)^{\frac{1}{4}} \left(1 - \frac{3}{8N_F} + O(N_F^{-2})\right) \exp(-N_F/8).$$

⁴SCM and T. Hohage (2017). *SIAM Journal of Applied Mathematics* **77**(2): 384–408.

Well-Posedness and Stability Result

Theorem 4 (Well-posedness and stability estimate for $IP2^4$)

Let $A := \{h \in L^2(\mathbb{R}^m) : \text{supp}(h) \subset \Omega\}$ with supporting domain Ω given by a stripe of width 1, w.l.o.g. $\Omega := [-\frac{1}{2}; \frac{1}{2}] \times \mathbb{R}^{m-1}$. Then

$$\|Th\| \geq C_{IP2}(\Omega, N_F) \|h\| \quad \text{for all } h \in A,$$

where the stability constant $C_{IP2}(\Omega, N_F) > 0$ satisfies the estimate

$$C_{IP2}(\Omega, N_F) \geq (2\pi N_F)^{\frac{1}{4}} \left(1 - \frac{3}{8N_F} + O(N_F^{-2})\right) \exp(-N_F/8).$$

Proof:

- By rectangular geometry of Ω , the Fourier transform factorizes:

$$\begin{aligned} C_{IP2}^2 &= \inf_{h \in L^2(\Omega), \|h\|=1} \left\| \mathcal{F}(h)|_{\Omega_F^c} \right\|^2 = \inf_{h \in L^2(\Omega), \|h\|=1} \left\| \mathcal{F}^{(m)} \otimes \dots \otimes \mathcal{F}^{(1)}(h)|_{\Omega_F^c} \right\|^2 \\ &= 1 - \sup_{h \in L^2\left(\left[-\frac{1}{2}; \frac{1}{2}\right]\right), \|h\|=1} \left\| \mathcal{F}(h)|_{[-N_F/4; N_F/4]} \right\|^2 \end{aligned}$$

⁴SCM and T. Hohage (2017). *SIAM Journal of Applied Mathematics* **77**(2): 384—408.

Well-Posedness and Stability Result

Theorem 4 (Well-posedness and stability estimate for $\text{IP}2^4$)

Let $A := \{h \in L^2(\mathbb{R}^m) : \text{supp}(h) \subset \Omega\}$ with supporting domain Ω given by a stripe of width 1, w.l.o.g. $\Omega := [-\frac{1}{2}; \frac{1}{2}] \times \mathbb{R}^{m-1}$. Then

$$\|Th\| \geq C_{\text{IP}2}(\Omega, N_F) \|h\| \quad \text{for all } h \in A,$$

where the stability constant $C_{\text{IP}2}(\Omega, N_F) > 0$ satisfies the estimate

$$C_{\text{IP}2}(\Omega, N_F) \geq (2\pi N_F)^{\frac{1}{4}} \left(1 - \frac{3}{8N_F} + O(N_F^{-2})\right) \exp(-N_F/8).$$

Proof:

- By rectangular geometry of Ω , the Fourier transform factorizes:

$$\begin{aligned} C_{\text{IP}2}^2 &= \inf_{h \in L^2(\Omega), \|h\|=1} \left\| \mathcal{F}(h)|_{\Omega_F^c} \right\|^2 = \inf_{h \in L^2(\Omega), \|h\|=1} \left\| \mathcal{F}^{(m)} \otimes \dots \otimes \mathcal{F}^{(1)}(h)|_{\Omega_F^c} \right\|^2 \\ &= 1 - \sup_{h \in L^2([-\frac{1}{2}; \frac{1}{2}]), \|h\|=1} \left\| \mathcal{F}(h)|_{[-N_F/4; N_F/4]} \right\|^2 \end{aligned}$$

- Need max singular value of 1D-operator $\mathcal{F}_F : h \mapsto \mathcal{F}(h)|_{[-N_F/4; N_F/4]}$

⁴SCM and T. Hohage (2017). *SIAM Journal of Applied Mathematics* **77**(2): 384–408.

Well-Posedness and Stability Result (continued)

- By convolution thm: $\mathcal{F}_F^* \mathcal{F}_F : L^2([-1/2; 1/2]) \rightarrow L^2([-1/2; 1/2])$ is of the form

$$\begin{aligned}\mathcal{F}_F^* \mathcal{F}_F(h) &= \mathbf{1}_{[-1/2; 1/2]} \cdot \mathcal{F}^{-1}(\mathbf{1}_{[-N_F/4; N_F/4]} \cdot \mathcal{F}(h)) \\ &= \int_{-1/2}^{1/2} \frac{\sin(2c(\cdot - y))}{\pi(\cdot - y)} h(y) dy =: K_c h, \quad c = N_F/8\end{aligned}$$

Well-Posedness and Stability Result (continued)

- ▶ By convolution thm: $\mathcal{F}_F^* \mathcal{F}_F : L^2([-1/2; 1/2]) \rightarrow L^2([-1/2; 1/2])$ is of the form

$$\begin{aligned} \mathcal{F}_F^* \mathcal{F}_F(h) &= \mathbf{1}_{[-1/2; 1/2]} \cdot \mathcal{F}^{-1}(\mathbf{1}_{[-N_F/4; N_F/4]} \cdot \mathcal{F}(h)) \\ &= \int_{-1/2}^{1/2} \frac{\sin(2c(\cdot - y))}{\pi(\cdot - y)} h(y) dy =: K_c h, \quad c = N_F/8 \end{aligned}$$

- ▶ Eigenvalues $\lambda_0 > \lambda_1 > \dots$ of compact selfadjoint integral operators K_c asymptotically characterized for $c \rightarrow \infty$ ⁵:

$$1 - \lambda_n = \frac{2^{3n+2} \pi^{1/2} c^{n+1/2}}{n!} \left(1 - \frac{6n^2 - 2n + 3}{32c} + O\left(\frac{1}{c^2}\right) \right) \exp(-2c)$$

⁵Slepian, D and Sonnenblick, E (1965). *Bell System Technical Journal* **44**(8): 1745–1759.

Well-Posedness and Stability Result (continued)

- ▶ By convolution thm: $\mathcal{F}_F^* \mathcal{F}_F : L^2([-1/2; 1/2]) \rightarrow L^2([-1/2; 1/2])$ is of the form

$$\begin{aligned} \mathcal{F}_F^* \mathcal{F}_F(h) &= \mathbf{1}_{[-1/2; 1/2]} \cdot \mathcal{F}^{-1}(\mathbf{1}_{[-N_F/4; N_F/4]} \cdot \mathcal{F}(h)) \\ &= \int_{-1/2}^{1/2} \frac{\sin(2c(\cdot - y))}{\pi(\cdot - y)} h(y) dy =: K_c h, \quad c = N_F/8 \end{aligned}$$

- ▶ Eigenvalues $\lambda_0 > \lambda_1 > \dots$ of compact selfadjoint integral operators K_c asymptotically characterized for $c \rightarrow \infty$ ⁵:

$$1 - \lambda_n = \frac{2^{3n+2} \pi^{1/2} c^{n+1/2}}{n!} \left(1 - \frac{6n^2 - 2n + 3}{32c} + O\left(\frac{1}{c^2}\right) \right) \exp(-2c)$$

- ▶ $C_{IP2}(\Omega, N_F)^2 \geq 1 - \lambda_0$

□

⁵Slepian, D and Sonnenblick, E (1965). *Bell System Technical Journal* **44**(8): 1745–1759.

Well-Posedness and Stability Result (continued)

- ▶ By convolution thm: $\mathcal{F}_F^* \mathcal{F}_F : L^2([-1/2; 1/2]) \rightarrow L^2([-1/2; 1/2])$ is of the form

$$\begin{aligned} \mathcal{F}_F^* \mathcal{F}_F(h) &= \mathbf{1}_{[-1/2; 1/2]} \cdot \mathcal{F}^{-1}(\mathbf{1}_{[-N_F/4; N_F/4]} \cdot \mathcal{F}(h)) \\ &= \int_{-1/2}^{1/2} \frac{\sin(2c(\cdot - y))}{\pi(\cdot - y)} h(y) dy =: K_c h, \quad c = N_F/8 \end{aligned}$$

- ▶ Eigenvalues $\lambda_0 > \lambda_1 > \dots$ of compact selfadjoint integral operators K_c asymptotically characterized for $c \rightarrow \infty^5$:

$$1 - \lambda_n = \frac{2^{3n+2} \pi^{1/2} c^{n+1/2}}{n!} \left(1 - \frac{6n^2 - 2n + 3}{32c} + O\left(\frac{1}{c^2}\right) \right) \exp(-2c)$$

- ▶ $C_{IP2}(\Omega, N_F)^2 \geq 1 - \lambda_0$ □

Remark 5

Proof relates least stable modes of T to low-order *prolate spheroidal wave functions* (scaled by $n_F^{1/2}$) \rightsquigarrow *low-frequency instabilities*.

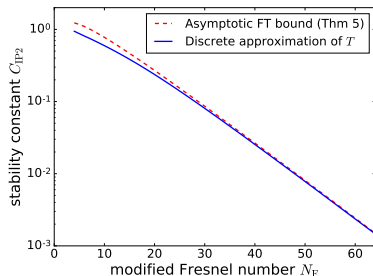
⁵Slepian, D and Sonnenblick, E (1965). *Bell System Technical Journal* **44**(8): 1745–1759.

Numerical Validation

- **Optimality problem:** How lossy is the restriction $Th \mapsto \mathcal{D}^2(h)|_{\Omega^c}$?

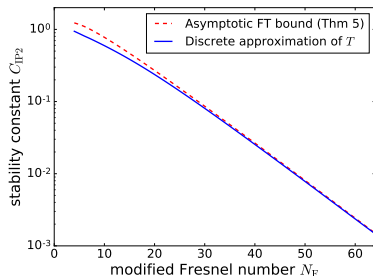
Numerical Validation

- **Optimality problem:** How lossy is the restriction $Th \mapsto \mathcal{D}^2(h)|_{\Omega^c}$?
- Compare analytical bound (Thm 4) for C_{IP_2} to minimum singular value of discretized operator T in 1D



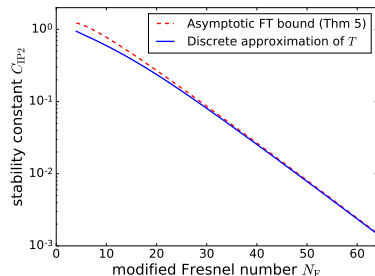
Numerical Validation

- **Optimality problem:** How lossy is the restriction $Th \mapsto \mathcal{D}^2(h)|_{\Omega^c}$?
- Compare analytical bound (Thm 4) for C_{IP_2} to minimum singular value of discretized operator T in 1D
- ▶ *Excellent agreement* of analytical reduction with full forward model



Numerical Validation

- **Optimality problem:** How lossy is the restriction $Th \mapsto \mathcal{D}^2(h)|_{\Omega^c}$?
- Compare analytical bound (Thm 4) for C_{IP2} to minimum singular value of discretized operator T in 1D
- ▶ *Excellent agreement* of analytical reduction with full forward model

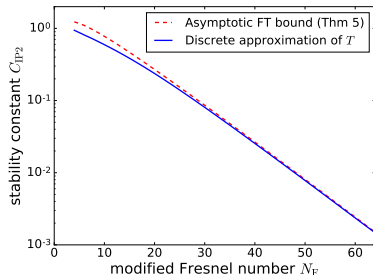


Well-posedness \Rightarrow stable image reconstruction?

- Well-posed but *ill-conditioned* for general complex-valued images

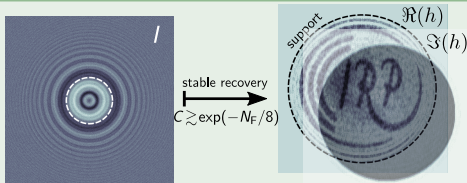
Numerical Validation

- **Optimality problem:** How lossy is the restriction $Th \mapsto \mathcal{D}^2(h)|_{\Omega^c}$?
- Compare analytical bound (Thm 4) for C_{IP2} to minimum singular value of discretized operator T in 1D
- ▶ *Excellent agreement* of analytical reduction with full forward model



Well-posedness \Rightarrow stable image reconstruction?

- Well-posed but *ill-conditioned* for general complex-valued images
- Reconstruction feasible iff $N_F \lesssim 100$ ⁶



⁶SCM, Bartels M, Krenkel M, Salditt T, and Hohage T. (2016). *Optics Express* **24**(6): 6490-6506.

Extensions and Reconstructions

Homogeneous Objects

Homogeneity constraint:

Assume $h = -ie^{-i\alpha}\varphi$ with φ real-valued (\rightsquigarrow e.g. *non-absorbing* objects)

$$\Rightarrow Th = 2\mathcal{F}^{-1}\left(s_\alpha \cdot \mathcal{F}(\varphi)\right) =: S\varphi, \quad s_\alpha(\xi) = \sin\left(\frac{\xi^2}{2N_F} + \alpha\right)$$

Homogeneous Objects

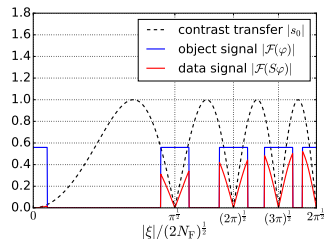
Homogeneity constraint:

Assume $h = -ie^{-i\alpha}\varphi$ with φ real-valued (\rightsquigarrow e.g. *non-absorbing* objects)

$$\Rightarrow Th = 2\mathcal{F}^{-1}\left(s_\alpha \cdot \mathcal{F}(\varphi)\right) =: S\varphi, \quad s_\alpha(\xi) = \sin\left(\frac{\xi^2}{2N_F} + \alpha\right)$$

Stability analysis:

- Forward operator is Fourier-multiplier
 \rightsquigarrow unstable around zeros of s_α



Homogeneous Objects

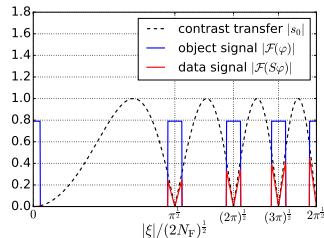
Homogeneity constraint:

Assume $h = -ie^{-i\alpha}\varphi$ with φ real-valued (\rightsquigarrow e.g. *non-absorbing* objects)

$$\Rightarrow Th = 2\mathcal{F}^{-1}\left(s_\alpha \cdot \mathcal{F}(\varphi)\right) =: S\varphi, \quad s_\alpha(\xi) = \sin\left(\frac{\xi^2}{2N_F} + \alpha\right)$$

Stability analysis:

- Forward operator is Fourier-multiplier
 \rightsquigarrow unstable around zeros of s_α



Homogeneous Objects

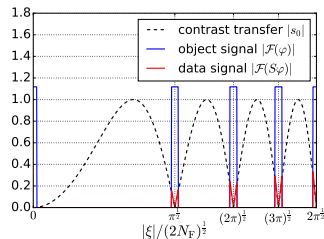
Homogeneity constraint:

Assume $h = -ie^{-i\alpha}\varphi$ with φ real-valued (\rightsquigarrow e.g. *non-absorbing* objects)

$$\Rightarrow Th = 2\mathcal{F}^{-1}\left(s_\alpha \cdot \mathcal{F}(\varphi)\right) =: S\varphi, \quad s_\alpha(\xi) = \sin\left(\frac{\xi^2}{2N_F} + \alpha\right)$$

Stability analysis:

- Forward operator is Fourier-multiplier
 \rightsquigarrow unstable around zeros of s_α



Homogeneous Objects

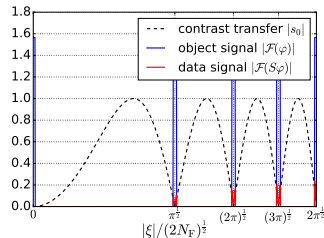
Homogeneity constraint:

Assume $h = -ie^{-i\alpha}\varphi$ with φ real-valued (\rightsquigarrow e.g. *non-absorbing* objects)

$$\Rightarrow Th = 2\mathcal{F}^{-1}\left(s_\alpha \cdot \mathcal{F}(\varphi)\right) =: S\varphi, \quad s_\alpha(\xi) = \sin\left(\frac{\xi^2}{2N_F} + \alpha\right)$$

Stability analysis:

- Forward operator is Fourier-multiplier
 \rightsquigarrow unstable around zeros of s_α



Homogeneous Objects

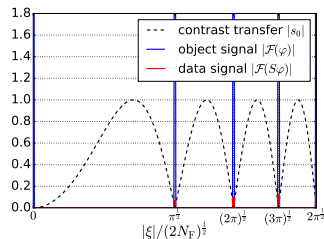
Homogeneity constraint:

Assume $h = -ie^{-i\alpha}\varphi$ with φ real-valued (\rightsquigarrow e.g. *non-absorbing* objects)

$$\Rightarrow Th = 2\mathcal{F}^{-1}\left(s_\alpha \cdot \mathcal{F}(\varphi)\right) =: S\varphi, \quad s_\alpha(\xi) = \sin\left(\frac{\xi^2}{2N_F} + \alpha\right)$$

Stability analysis:

- Forward operator is Fourier-multiplier
 \rightsquigarrow unstable around zeros of s_α



Homogeneous Objects

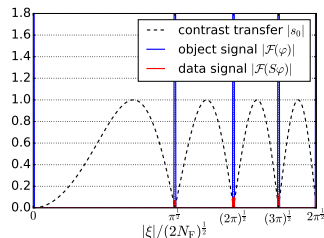
Homogeneity constraint:

Assume $h = -ie^{-i\alpha}\varphi$ with φ real-valued (\rightsquigarrow e.g. *non-absorbing* objects)

$$\Rightarrow Th = 2\mathcal{F}^{-1}\left(s_\alpha \cdot \mathcal{F}(\varphi)\right) =: S\varphi, \quad s_\alpha(\xi) = \sin\left(\frac{\xi^2}{2N_F} + \alpha\right)$$

Stability analysis:

- Forward operator is Fourier-multiplier
 \rightsquigarrow unstable around zeros of s_α
- Constraint $\text{supp}(\varphi) \subset \overline{B(0, 1/2)}$ enforces smooth FT: $\|\nabla\mathcal{F}(\varphi)\| = \|\mathbf{x}\varphi\| \leq \frac{1}{2}\|\varphi\|$



Homogeneous Objects

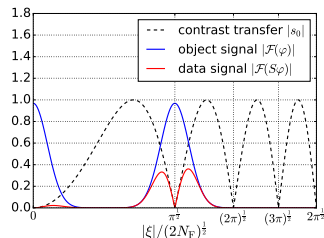
Homogeneity constraint:

Assume $h = -ie^{-i\alpha}\varphi$ with φ real-valued (\rightsquigarrow e.g. *non-absorbing* objects)

$$\Rightarrow Th = 2\mathcal{F}^{-1}\left(s_\alpha \cdot \mathcal{F}(\varphi)\right) =: S\varphi, \quad s_\alpha(\xi) = \sin\left(\frac{\xi^2}{2N_F} + \alpha\right)$$

Stability analysis:

- Forward operator is Fourier-multiplier
 \rightsquigarrow unstable around zeros of s_α
- Constraint $\text{supp}(\varphi) \subset \overline{B(0, 1/2)}$ enforces smooth FT: $\|\nabla\mathcal{F}(\varphi)\| = \|\mathbf{x}\varphi\| \leq \frac{1}{2}\|\varphi\|$
- Finitely sharp peaks of $\mathcal{F}(\varphi) \rightsquigarrow$ *stability*



Homogeneous Objects

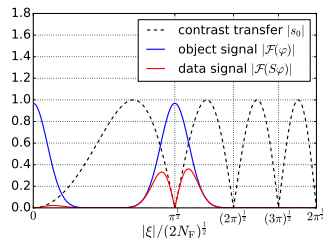
Homogeneity constraint:

Assume $h = -ie^{-i\alpha}\varphi$ with φ real-valued (\rightsquigarrow e.g. *non-absorbing* objects)

$$\Rightarrow Th = 2\mathcal{F}^{-1}\left(s_\alpha \cdot \mathcal{F}(\varphi)\right) =: S\varphi, \quad s_\alpha(\xi) = \sin\left(\frac{\xi^2}{2N_F} + \alpha\right)$$

Stability analysis:

- Forward operator is Fourier-multiplier
 \rightsquigarrow unstable around zeros of s_α
- Constraint $\text{supp}(\varphi) \subset \overline{B(0, 1/2)}$ enforces smooth FT: $\|\nabla\mathcal{F}(\varphi)\| = \|\mathbf{x}\varphi\| \leq \frac{1}{2}\|\varphi\|$
- Finitely sharp peaks of $\mathcal{F}(\varphi) \rightsquigarrow$ *stability*



Theorem 6 (Improved stability under homogeneity constraint⁴)

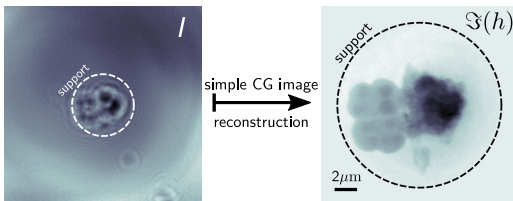
Let $h = -ie^{-i\alpha}\varphi$ with $\varphi \in L^2(\mathbb{R}^m, \mathbb{R})$ and $\text{supp}(h) \subset \overline{B(0, 1/2)}$. Then

$$\|Th\| \geq \max\left\{\min\left\{c_1, c_2 N_F^{-1}\right\}, \min\left\{c_3 \alpha, c_4 N_F^{-\frac{1}{2}}\right\}\right\} \|h\| \quad (c_j > 0)$$

⁴SCM and T. Hohage (2017). *SIAM Journal of Applied Mathematics* **77**(2): 384–408.

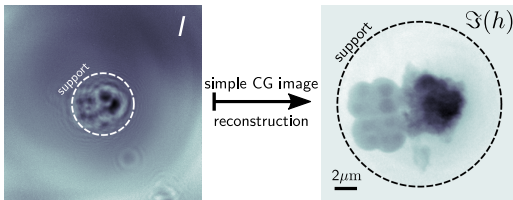
Reconstructions from Experimental Data

1 Non-absorbing object: Well-posed + well-conditioned (for $N_F \lesssim 100$)



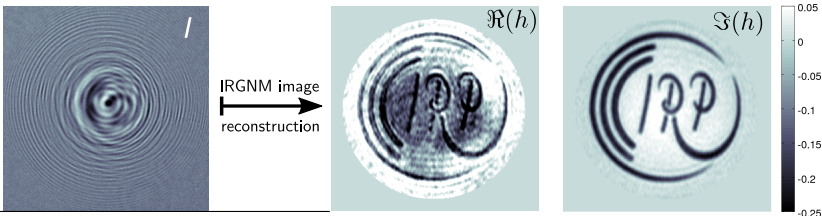
Reconstructions from Experimental Data

1 Non-absorbing object: Well-posed + well-conditioned (for $N_F \lesssim 100$)



2 General object⁶: severely ill-conditioned \rightsquigarrow regularize

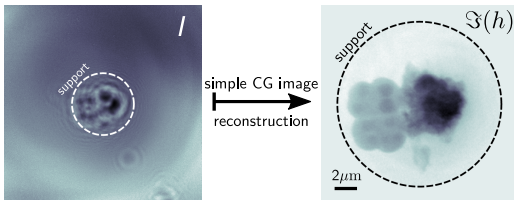
$$h_{k+1} = \operatorname{argmin}_{h \in L^2(\Omega)} \|F(h_k) + F'[h_k](h - h_k) - I\|_{L^2}^2 + \alpha \|h\|_{H^s}^2 +$$



⁶SCM, Bartels M, Krenkel M, Salditt T, and Hohage T. (2016). *Optics Express* **24**(6): 6490-6506.

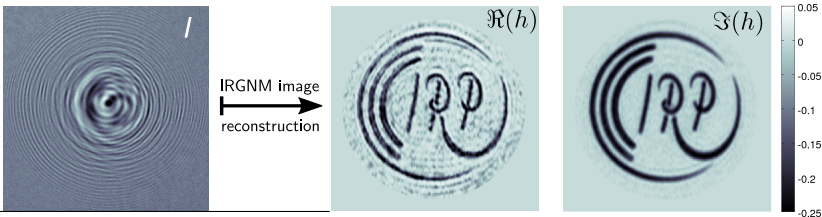
Reconstructions from Experimental Data

1 Non-absorbing object: Well-posed + well-conditioned (for $N_F \lesssim 100$)



2 General object⁶: severely ill-conditioned \rightsquigarrow regularize + constraints

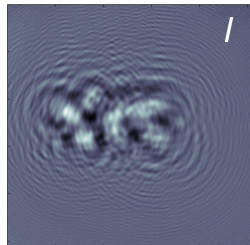
$$h_{k+1} = \operatorname{argmin}_{h \in L^2(\Omega)} \|F(h_k) + F'[h_k](h - h_k) - I\|_{L^2}^2 + \alpha \|h\|_{H^s}^2 + \mathcal{P}_{\mathcal{C}_-}(h)$$



⁶SCM, Bartels M, Krenkel M, Salditt T, and Hohage T. (2016). *Optics Express* **24**(6): 6490-6506.

Finite Detectors

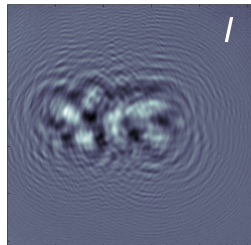
- Intensity I measured within bounded detector domain $D \subset \mathbb{R}^2$



Finite Detectors

- Intensity I measured within bounded detector domain $D \subset \mathbb{R}^2$
- Propagator \mathcal{D} is arbitrarily nonlocal:

$$\mathcal{D}\left(\underbrace{\delta_0}_{\text{supp}=\{0\}}\right)(\mathbf{x}) \propto \underbrace{\exp(-iN_F \mathbf{x}^2/2)}_{\text{supp}=\mathbb{R}^2}$$

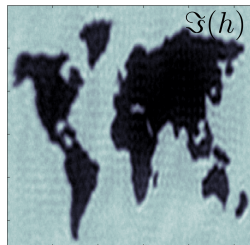
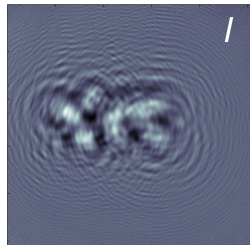


Finite Detectors

- Intensity I measured within bounded detector domain $D \subset \mathbb{R}^2$
- Propagator \mathcal{D} is arbitrarily nonlocal:

$$\mathcal{D}\left(\underbrace{\delta_0}_{\text{supp}=\{0\}}\right)(\mathbf{x}) \propto \underbrace{\exp(-iN_F \mathbf{x}^2/2)}_{\text{supp}=\mathbb{R}^2}$$

- ▶ Problem $I|_D \mapsto h$ is exponentially ill-posed:
infinitely sharp structures cannot be resolved

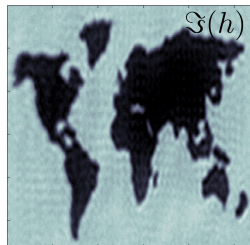
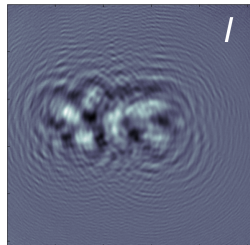


Finite Detectors

- Intensity I measured within bounded detector domain $D \subset \mathbb{R}^2$
- Propagator \mathcal{D} is arbitrarily nonlocal:

$$\mathcal{D}\left(\underbrace{\delta_0}_{\text{supp}=\{0\}}\right)(\mathbf{x}) \propto \underbrace{\exp(-iN_F \mathbf{x}^2/2)}_{\text{supp}=\mathbb{R}^2}$$

- ▶ Problem $I|_D \mapsto h$ is exponentially ill-posed: infinitely sharp structures cannot be resolved
- ▶ Stability restored for $h \in L^2(\Omega) \cap \mathcal{S}_r = \left\{ \text{bilinear splines of resolution } r \sim \frac{1}{\text{dist}(\partial D, \Omega) \cdot N_F} \right\}$

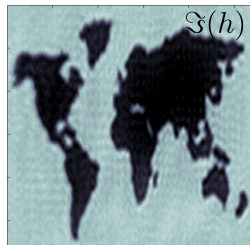
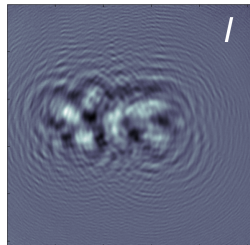


Finite Detectors

- Intensity I measured within bounded detector domain $D \subset \mathbb{R}^2$
- Propagator \mathcal{D} is arbitrarily nonlocal:

$$\mathcal{D}\left(\underbrace{\delta_0}_{\text{supp}=\{0\}}\right)(\mathbf{x}) \propto \underbrace{\exp(-iN_F \mathbf{x}^2/2)}_{\text{supp}=\mathbb{R}^2}$$

- ▶ Problem $I|_D \mapsto h$ is exponentially ill-posed: infinitely sharp structures cannot be resolved
- ▶ Stability restored for $h \in L^2(\Omega) \cap \mathcal{S}_r = \{ \text{bilinear splines of resolution } r \sim \frac{1}{\text{dist}(\partial D, \Omega) \cdot N_F} \}$



Analysis:

- Gaussian-smoothed objects $h_\sigma = p_\sigma * h$

$$\mathcal{D}(h_\sigma) = \mathcal{D}(p_\sigma) * h = \underbrace{(u \cdot p_{\tilde{\sigma}})}_{\text{localized}} * h, \quad \tilde{\sigma} \sim 1/(\sigma N_F)$$
- Exploit that $\|p_\sigma * h\| \geq \frac{1}{2} \|h\|$ for $h \in \mathcal{S}_r, r \gtrsim \sigma$

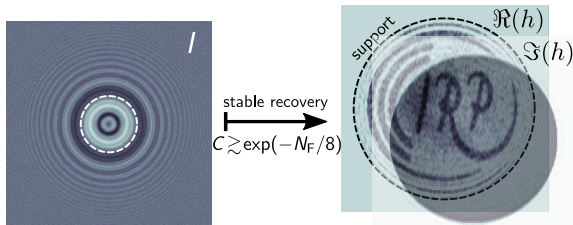
Conclusions

Summary

- X-ray phase contrast enables nanoscale imaging of soft-tissue

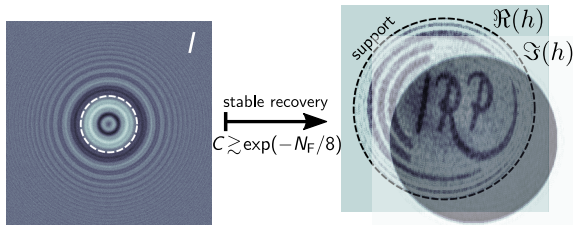
Summary

- X-ray phase contrast enables nanoscale imaging of soft-tissue
- Established stability of linearized model under support constraints
 \rightsquigarrow *well-posed* phase retrieval problem



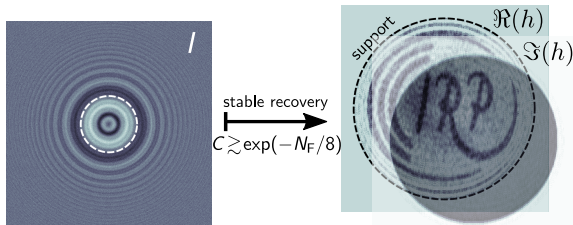
Summary

- X-ray phase contrast enables nanoscale imaging of soft-tissue
- Established stability of linearized model under support constraints
 \rightsquigarrow *well-posed* phase retrieval problem
- Analysis: Reduction to reconstruction from incomplete Fourier data



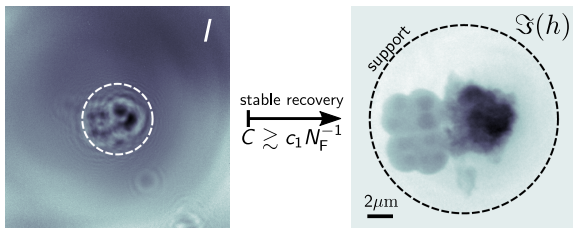
Summary

- X-ray phase contrast enables nanoscale imaging of soft-tissue
- Established stability of linearized model under support constraints
 \rightsquigarrow *well-posed* phase retrieval problem
- Analysis: Reduction to reconstruction from incomplete Fourier data
- General stability bound $C_{IP2} \gtrsim \exp(-N_F/8)$ supported by numerical results + correct prediction of *low-frequency instabilities*



Summary

- X-ray phase contrast enables nanoscale imaging of soft-tissue
- Established stability of linearized model under support constraints
 \rightsquigarrow *well-posed* phase retrieval problem
- Analysis: Reduction to reconstruction from incomplete Fourier data
- General stability bound $C_{IP2} \gtrsim \exp(-N_F/8)$ supported by numerical results + correct prediction of *low-frequency instabilities*
- Improved stability $C_{IP2} \gtrsim N_F^{-1}$ under homogeneity constraint (non-absorbing objects) **or** for *two* diffraction patterns I_1, I_2



References I



Gabor, D. et al. (1948).

A new microscopic principle.

Nature, 161(4098):777–778.



Jonas, P. and Louis, A. (2004).

Phase contrast tomography using holographic measurements.

Inverse Problems, 20(1):75.



Maretzke, S. (2015).

A uniqueness result for propagation-based phase contrast imaging from a single measurement.

Inverse Problems, 31:065003.

References II



Maretzke, S., Bartels, M., Krenkel, M., Salditt, T., and Hohage, T. (2016).

Regularized Newton methods for X-ray phase contrast and general imaging problems.

Optics Express, 24(6):6490–6506.



Maretzke, S. and Hohage, T. (2017).

Stability estimates for linearized near-field phase retrieval in X-ray phase contrast imaging.

SIAM Journal on Applied Mathematics, 77:384—408.



Salditt, T., Osterhoff, M., Krenkel, M., Wilke, R. N., Priebe, M., Bartels, M., Kalbfleisch, S., and Sprung, M. (2015).

Compound focusing mirror and x-ray waveguide optics for coherent imaging and nano-diffraction.

Journal of synchrotron radiation, 22(4):867–878.

References III



Slepian, D. and Sonnenblick, E. (1965).

Eigenvalues associated with prolate spheroidal wave functions of zero order.

Bell System Technical Journal, 44(8):1745–1759.